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Abstract.

The demand for rapid procedures to solve Poisson's equation has lead to the development of a direct method of solution involving Fourier analysis which can solve Poisson's equation in a square region covered by a 48 x 48 mesh in 0.9 seconds on the IBM 7090. This compares favorably with the best iterative methods which would require about 10 seconds to solve the same problem.

The method is applicable to rectangular regions with simple boundary conditions and the maximum observed error in the potential for several random charge distributions is 5×10^{-7} of the maximum potential change in the region.

1. Introduction.

In many engineering problems concerning plasmas, electron tubes and ion guns, it is desired to follow the motion of numerous electrostatically interacting charged particles in two dimensions. If the region involved is divided into a large number -of cells, and the velocity and position of each charged particle is recorded, then this simulation of space charge flow may be performed stepwise in time as follows:

*First presented to the Denver meeting of the A.C.M. August 1963. Applications of the method to the Computer Simulation of Plasma phenomina have been reported to the San Diego meeting of the A.P.S. November 1963 and to the Plasma Instabilities meeting at Berkeley April 1964.

1. The charge distribution;

At the beginning of each time step the position of each particle is examined and the charge of each particle is associated with the center of the cell in which the particle resides.

2. The potential;

The charge distribution found in step 1 is used as the source term or right-hand side of Poisson% equation, the solution of which gives the electrostatic potential in the region,

3. The acceleration,

The potential distribution found in step 2 is differenced to give an approximation to the electrostatic field acting on each particle, This field is then allowed to accelerate each particle individually for a short time interval. The new position and velocity of each particle is recorded and the cycle repeats at step 1. The description is thus analogous to the projection of a motion picture.

For such a simulation to be useful it is necessary to follow several thousand particles through several hundred time-steps and this means that the overall cycle time must be reduced to a few seconds or less.

The acceleration of all the particles is a simple calculation and can be performed in about-a second on the IBM 7090*. The solution of Poisson's partial differential equation in step 2 is more difficult but it is clear that the solution must be obtained in about the same time if the simulation is to be useful.

* Computation times given in this paper will be for this machine except where specified,

Hithertoo the tendency has been to use iterative methods to solve such an elliptic equation. Theoretical estimates of the computing time for the best iterative methods,namely the two line cyclic Chebyshev (2LCC) and Alternating Direction Implicite (ADI) methods, have been made which compare well with the experimental results of Hageman [1] and Price and Varga [2].

These lead to solution times of 10 secs, 30 secs and 60 secs for respectively ADI, 2LCC and SOR methods when applied to a 48 × 48 square mesh and an error reduction of 10^{-6}.

These solution times are thus roughly 10 times too slow for this application.

The iterative methods of solution named above are very general and can be used to solve Poisson's equation in systems with complicated electrode shapes and boundary conditions. In Plasma applications however, where the behavior of the space charge distribution is of primary importance, it is often permissible to simplify the boundary conditions in order to obtain a faster solution.

In this paper we describe an alternative direct method of solution which takes advantage of this simplification,is applicable to a certain class of important problems,and is 10 times faster than the best iterative methods so far reported.,

2. Motivation and Discussion.

The problem to be discussed is the solution of Poisson's equation in a rectangular domain where the boundary conditions are given on the perimeter of the domain only. The boundary conditions may be Dirichlet, Neumann or periodic (combination being permitted provided that the same type of condition pertains along the total length of any side). The method shows to best advantage in (x,y) cordinates and we shall consider this case and take the boundary conditions to be zero potential around the perimeter.

We have

$$\frac{\partial^2\varphi(x,y)}{\partial x^2} + \frac{\partial^2\varphi(x,y)}{\partial y^2} = \rho(x,y) \qquad \begin{array}{l} 0 \leq x \leq \ell \\ 0 \leq y \leq m \end{array} \qquad (1)$$

$$\varphi(x,y) = 0 \qquad \text{for} \quad x = 0,\ a \quad \text{or}\ y = 0,\ m$$

2.1 , Fourier Analysis.

The boundary conditions allow $\varphi(x,y)$ to be expanded in a Fourier series in either the x direction, y direction or as a double Fourier series in both directions A double Fourier expansion was suggested as long ago as 1952 by Hyman [7] and is essentially the method of Tensor Products reported recently by Lynch et al [8]. However the determination of Fourier coefficients is a time consuming job on a computer and we have found that the fastest computer programme is obtained if we expand in only one direction and choose this to be shortest. Let this be the x direction then the expansion is

$$\varphi(x,y) = \sum_k \bar{\varphi}^k (y) \operatorname{Sin} \frac{\pi k x}{\ell} \qquad (2)$$

and similarly for $\rho(x,y)$ where $\bar{\varphi}^k$ (y) is the Fourier amplitude of the kth harmonic.

On substituting (2) into the partial differential equation (1) and using the orthogonal properties of the Sine functions we obtain a set of ordinary differential equations relating the Fourier amplitudes of $\varphi(x,y)$ and $\rho(x,y)$

$$\frac{d^2\bar{\varphi}^k(y)}{dy^2} - \left(\frac{\pi k}{L}\right)^2 \bar{\varphi}^k (y) = \bar{\rho}^k (y) \qquad (3)$$

In the continuous case an infinite number of harmonic amplitudes are required in the representation of $\varphi(x,y)$. However when we perform the finite analogue of the expansion (2) to express the value of $\varphi(x,y)$ at a discrete number of mesh points only, we find the number of harmonics required for the exact representation of the mesh function is equal to the numberof mesh points (see for example Jeffreys and Jeffreys [6] paragraph 14.01).

Due to the fact that the Sine functions satisfy the boundary conditions and are the eigenfunctions of the differential operator in equation (1), the ordinary differential equations (3) for each harmonic are independent of each other. This change of a partial differential equation into a set of independent ordinary differential equations is the first crucial simplification of the method. It can only be carried out in certain simple geometrical situations when, for example, the external boundaries are parallel to the coordinate axes and the boundary conditions are of the type mentioned above. The presence of any internal conductors for example immediately couples the harmonics in equation (3) and makes the method as it stands impractical. However a modification of this direct method is being investigated which will allow the inclusion of interior boundaries and is suitable for cases where Poisson's equation is to be solved repeatedly for different space charge distributions but with fixed interior electrode surfaces. Some preliminary calculation, done once only, is required after which it is expected that the solution time will be no more than doubled.

2.2 Tridiagonal systems.

The ordinary differential equations (3), which in the finite analogue become a tridiagonal matrix equation, can be solved in a variety of ways. Our experience has been that the best technique depends on the boundary conditions imposed.

In the case that the potential and therefore $\bar{\varphi}^k(y)$ has prescribed values at y = 0, m the method of Gauss Elimination in the neat form as given by Varga [9] and others is suitable and may be used for any number of mesh points. Gauss elimination is an inefficient method to use if the boundary conditions are periodic and a new technique of 'recursive cyclic reduction' has been developed for this case which is particularly neat if the number of mesh points is of the form 2^p or 3×2^p (see section 6). This does not seem a severe restriction considering the resulting increase in computing speed. Indeed 'recursive cyclic reduction' may be applied to the Dirichlet boundary conditions for these special numbers of mesh points and has the advantage over Gauss Elimination that it does not require the precomputation and storage of the auxiliary vector ω (see Varga [9] p. 195).

An interesting and quick method of solution has been suggested by 0. Buneman for the case that $\bar{\varphi}^k(0)$ is given and we have an open ended Neumann condition that

$$\frac{d\bar{\varphi}^k}{dy} = \bar{\varphi}^k = 0 \quad \text{at} \quad y = \infty \tag{4}$$

In this case the equations (3) or their finite difference analogue may be factorized as follows,

$$\left\{\frac{d}{dy} - (\frac{\pi k}{L})\right\} \left\{\frac{d}{dy} + (\frac{\pi k}{L})\right\} \bar{\varphi}^k (y) = \bar{\rho}^k (y) \tag{5}$$

introducing the auxiliary function $\bar{\psi}^k$ (y) defined by

$$\left\{\frac{d}{dy} - \left(\frac{\pi k}{L}\right)\right\} \bar{\psi}^{k}(y) = \bar{\rho}^{k}(y) \qquad (6)$$

we have

$$\left\{\frac{d}{dy} + \left(\frac{\pi k}{L}\right)\right\} \bar{\varphi}^{k}(y) = \bar{\psi}^{k}(y) \qquad (7)$$

Applying the condition (4) to (7) we see that $\bar{\psi}^{k}(\infty) = 0$. Integrating equation (6) inwards from infinity we see that $\bar{\psi}^{k}(y) = 0$ until the first charge is encountered, at $y = \hat{y}$ say. In practice therefore (6) is integrated only from $y = \hat{y}$ to $y = 0$ yielding $\bar{\psi}^{k}(\hat{y})$ to $\bar{\psi}^{k}(0)$. Knowing the right hand side, equation (-7) may be integrated from $y = 0$ to $y = \hat{y}$ starting with the known value of $\bar{\varphi}^{k}(0)$. This technique is known as the 'marching method' and if the march is performed in the directions given with the factorisation shown there is no build up of error due to the homogenous solutions of equations (6) and (7).

Having obtained $\bar{\varphi}^{k}(y)$ as the solution of equation (4) the potential $\varphi(y)$ is obtained by Fourier synthesis from equation (2).

Due to the reciprocity of the Finite Fourier analysis and synthesis the program for Fourier synthesis will have much in common if not all in common with the program for Fourier analysis.

Summarizing we see that the solution is obtained in three stages.

1. Fourier analysis of the charge distribution

$$\rho(x,y) \rightarrow \bar{\rho}^{k}(y)$$

2. Solution of k independent sets of ordinary differential equations or the corresponding tridiagonal matrix equations

$$\bar{\rho}^{k}(y) \rightarrow \bar{\varphi}^{k}(y)$$

3. Fourier synthesis of the potential distribution

$$\bar{\varphi}^k (y) \rightarrow \varphi(x,y)$$

2.3 Computer time.

If we examine the number of computer operations* required to perform this calculation the method does not, at first sight, seem particularly attractive. This is mainly due to the time required to perform the Analysis and Synthesis,as may be seen if we consider the domain of the solution to be spanned by an $(n \times n)$ mesh. For stage 1,on each of the n lines of constant y we must compute n Fourier components each of which require n operations giving a total of n^3 operations for the whole mesh. The solution of the n equations for one harmonic in stage 2 may be completed in the order of n operations giving a total of approximately n^2 operations for stage 2. Stage 3 of course also takes n^3 operations, As the conventional iterative methods will require of the order of n^2 operations per iterations it seems that the Fourier technique will only pay off if the number of iterations required is considerably larger than n. In a step by step simulation, when a good guess for the potential is available from the last time step,it seems quite likely that satisfactory convergence can be obtained in less than n iterations (n is typically 50 to 100). In this case no advantage has been obtained by the Fourier transformation and we have unnecessarilly restricted ourselves to certain simple types of boundary conditions,

* Here we mean a multiplication and the addition that usually accompanies it,

2.4 Simplifications.

Two further simplifications are, however, available in the Fourier method which completely reverse the above assessment. In the first place if a suitable number is chosen for n (such as 12, 24,48) there is a tremendous symmetry in the Sine functions which may be used to reduce the computing time for analysis and synthesis to about a tenth of the original estimate (see section 9b). Furthermore the two-cyclic nature of the finite difference equations allows one to replace the original n^2 equations involving all the points in the mesh to a set of $\frac{n^2}{2}$ slightly more complex equations involving only the points on the even lines of the mesh. This process known as cyclic-reduction may be done at the start and fortunately gives a set of revised equations which may also be solved by the Fourier method. The Fourier analysis and synthesis is then performed on only half the number of lines and computing time is reduced. The solution is completed by solving for the potential on the odd lines of the mesh directly from the known solution on the even lines. We have called this process odd/even reduction (see section 4).

2.5 Repeated reduction.

The revised equations on the even lines are themselves two-cyclic and it is attractive to consider whether it pays off to do another stage of cyclic reduction or even to perform cyclic reduction repeatedly until only a few lines of the mesh are left. The number of mesh points involved in each finite difference equation increases rapidly as the reduction process is continued and this means that **5** diagonal, 9 diagonal equation systems and worse must be solved when recovering the solutions on the omitted lines. These band equations can be solved by Fourier analysis and synthesis as well as by Gauss elimination or similar methods, and we have estimated that, is the case n = 48, systems wider than 5-diagonal are solved faster by Fourier analysis, If Fourier analysis is used to solve these equations it is easy to see that cyclic reduction has not significantly changed the process and the computing time will be unchanged. Our experience with the n = 48 case is that nothing is to be gained by more than one stage of cyclic reduction, This conclusion will be reversed for n large enough because the number of operations in the Gauss process is proportional to n compared with n^2 for solution by Fourier analysis.

The Fourier method as described above applied to (x,y) geometry can solve Poisson's equation of a (48 x 48) mesh in 0.9 sec with an error of about 10^{-6}. This time corresponds to about 10 computer operations per mesh point and if we estimate that an iterative will require at least 2 operations per point per iteration, we can see that an iterative method would have to converge in 5 iterations or less for it to be faster. It is hardly credible that any iterative method can achieve this.

Throughout the calculation new results may overwrite old and the storage required is very little more than the original mesh at n^2 points. With the aid of the results of section 9 we can extend the comparison made by Lynch in [8] of the total-number of arithmetic operations required to solve Poisson's equation on an (N x N) mesh:

SOR	Tensor Product	AD1	Fourier
$14N^3 \log N$	$4N^3$	$40N^2 \log^2 N$	$\frac{N^3}{5.5} + 9.5N^2$

On the basis of these estimates the Fourier method when applicable is always superior to SOR and the Tensor product methods and is superior to ADI for $N < 2500$ which includes all practical cases that can be solved on present day machines.

2.6 Other geometries.

(x,y) geometry is not always very realistic as it implies the existence of an infinite system in the z dimension., For many applications axially symmetric geometry on (r,z) coordinates is more appropriate, The Fourier method may be applied in these coordinates as described above if the Fourier analysis is performed in the z direction and the only change is that the tridiagonal system of equations in stage 2 now has variable coefficients. The cyclic reduction method is not suitable for such equations but the Gauss elimination method is as efficient in radial coordinates as in the x-coordinates. Thus if the z direction is the shortest there is no change in computing speed due to the change in the coordinate system. However if the z direction is the largest, as it frequently will be in electron tube work, the computing time will be increased and the alternative must be considered of performing a Bessel analysis and synthesis in the shorter r-direction. The Fourier method with Bessel analysis procedes in 3 stages as before however there is no symmetry in the Bessel analysis and the reduction of the number of operations by a factor of about 10 cannot be achieved as it could in the case of Fourier analysis. The odd/even reduction, however, may be performed as before. For z long enough a Bessel analysis in the shorter r-direction will be beneficial. Preliminary estimates suggest that Bessel analysis should only be performed if (z/r) is greater than about 8.

2.7 Generalization.

The basic principle of the Fourier method is the expansion of the solution in terms of the eigenfunctions of the Laplace operator for the problem. This principle can be used as a technique for solving certain types of matrix equations (see section 11.1) as well as a method for solving other types of linear differential equations (see section 11.2). The fact that there may be no analytic form for the eigenfunctions does not matter because these may be precomputed and stored in the computer. It is important however that the eigenfunctions have a large amount of symmetry. In the plasma problem considered in sections 3 to 10 the arithmetic operations are reduced by a factor of about 10 due to symmetrices in the Sine and Cosine functions which are the eigenfunctions. In the general case with the absense of this symmetry the computation time would be increased about 5 fold and the best iterative methods will probably be competitive.

Next we consider, in detail, the application of the Fourier method to a particular situation arising in a plasma study which uses a (48 x 48) mesh and report on the measured speed and accuracy of the solution. The boundary conditions being periodic are slightly different from the problem discussed above but the principle of the method is unchanged.

The Fourier method has also been successfully used in the Transient study of the Magnetron by Yu and Kooyers [10] using a (48 x 96) mesh with a solution time for Poisson% equation of 4 1/2 secs, and by Buneman and Wadhwa [ll] in an ion gun problem using a (24 x 100) mesh with a solution time of 2 secs. Both the above programs are in Fortran and could be speeded up significantly by writing in machine code.

3. The (48 x 48) Plasma Problem.

Consider a square region in (x,y) geometry covered by a square 48 x 48 mesh, with the boundary condition that the solution be periodically repeated in both the x and y directions,*

Using the usual 5-point difference approximation, Poisson's equation may be written in finite difference form as

$$\varphi_{i-1,j} + \varphi_{i+1,j} + \varphi_{i,j-1} + \varphi_{i,j+1} - 4\,\varphi_{i,j} = q_{i,j} \tag{8}$$

$$\text{for } i,j = 0,1,\ldots,(n-1) \qquad n = 48$$

where φ_{ij} is the potential at the (i,j) node of the mesh and q_{ij} is the charge associated with the (i,j) node of the mesh. The mesh numbering and interaction module for this approximation is shown in figure 1a.

The boundary conditions are

$$\left.\begin{aligned} \varphi_{i+kn,j+kn} &= \varphi_{i,j} \\ q_{i+kn,j+kn} &= q_{i,j} \end{aligned}\right\} \tag{9}$$

where k is any integer,

A convenient way of including these boundary conditions is to state that all indices are to be interpreted modulo n, and this will be assumed in the rest of this paper,

The equations (8) with boundary conditions (9) may be written in block matrix form as follows

* In order for the potential to be doubly periodic it is necessary for the total charge in the repeat square to be zero, We assume this to be the case.

$$B\,\underset{\sim}{\varphi} = \begin{pmatrix} A & I & 0\cdots 0 & I \\ I & A & I & \vdots \\ \vdots & & & 0 \\ 0 & I & A & I \\ I & 0\cdots 0 & I & A \end{pmatrix} \begin{pmatrix} \underset{\sim}{\varphi}_o \\ \underset{\sim}{\varphi}_1 \\ . \\ \underset{\sim}{\varphi}_{(n-1)} \end{pmatrix} = \begin{pmatrix} \underset{\sim}{q}_o \\ \underset{\sim}{q}_1 \\ \\ \underset{\sim}{q}_{(n-1)} \end{pmatrix} \qquad (10)$$

where

$$\underset{\sim}{\varphi}_j = \begin{pmatrix} \varphi_{o\,j} \\ \varphi_{1j} \\ \vdots \\ \varphi_{n-1,\,j} \end{pmatrix} \quad \text{and} \quad \underset{\sim}{q}_j = \begin{pmatrix} q_{o\,j} \\ q_{1j} \\ \vdots \\ q_{n-1,\,j} \end{pmatrix} \qquad (11)$$

and

$$A = \begin{pmatrix} -4 & 1 & 0\cdots 0 & & 1 \\ & & & & 0 \\ 1 & -4 & 1 & & \vdots \\ 0 & & & & 0 \\ \vdots & & & & \\ 0 & & 1 & -4 & 1 \\ 1 & 0\cdots 0 & & 1 & -4 \end{pmatrix} \qquad (12)$$

4. Odd/Even reduction.

The first step in the solution of equation (10) for the unknown potential on 48 lines of the mesh is the reduction of the problem to the solution of 24 more complicated equations for the unknown potential on the even numbered lines of the mesh only. After solving for the potential on the even lines the potential on the odd lines is obtained by exact interpolation as described in section 8.

Consider three neighboring equations from the matrix equation (10)

$$\left.\begin{aligned} \underset{\sim}{\varphi}_{j-2} + A\,\underset{\sim}{\varphi}_{j-1} + \underset{\sim}{\varphi}_j \qquad\qquad\qquad &= \underset{\sim}{q}_{j-1} \\ \underset{\sim}{\varphi}_{j-1} + A\,\underset{\sim}{\varphi}_j + \underset{\sim}{\varphi}_{j+1} \qquad &= \underset{\sim}{q}_j \\ \underset{\sim}{\varphi}_j + A\,\underset{\sim}{\varphi}_{j+1} + \underset{\sim}{\varphi}_{j+2} &= \underset{\sim}{q}_{j+1} \end{aligned}\right\} \qquad (13)$$

for $j = 2, 4, \ldots, n$ with the indices interpreted modulo 48.

By multiplying the second equation on the left by -A and adding we obtain

$$\underset{\sim}{\varphi}_{j-2} + (21 - A^2)\,\underset{\sim}{\varphi}_j + \underset{\sim}{\varphi}_{j+2} = \underset{\sim}{q}_{j-1} - A\underset{\sim}{q}_j + \underset{\sim}{q}_{j+1} \qquad (14)$$

for $j = 0, 2, \ldots, n-2$

The equations (14) are 24 equations for the even lines with a **7** point interaction module as shown in FIG lb. In expanded form they are

$$\varphi_{i,j-2} - \varphi_{i-2,j} + 8\,\varphi_{i-1,j} - 16\,\varphi_{i,j} + 8\,\varphi_{i+1,j} - \varphi_{i+2,j} + \varphi_{i,j+2}$$
$$= q_{i,j-1} - q_{i-1,j} + 4\,q_{i,j} - q_{i+1,j} + q_{i,j+1}$$

5. <u>Fourier Analysis.</u>

To solve equation (14) we first form a modified charge distribution on the even lines defined by

$$\underset{\sim}{q}^*_j = \underset{\sim}{q}_{j-1} - A\,\underset{\sim}{q}_j + \underset{\sim}{q}_{j+1} \qquad j = 0, 2, \ldots, 46 \qquad (15)$$

which in expanded form is

$$q^*_{i,j} = q_{i,j-1} - q_{i-1,j} + 4\,q_{i,j} - q_{i+1,j} + q_{i,j+1} \qquad (16)$$

for $i = 0, 1, \ldots .$ **47** , $j = 0, 2, \ldots,$ **46.**

From the point of view of machine storage the modified charge density on the even lines may overwrite the original charge density as it is formed.

Next the potential and charge distribution are expanded in Fourier components as follows:

$$\varphi_{i,j} = \frac{1}{2}\,\bar{\varphi}^{c}_{o,j} + \frac{1}{2}\,\bar{\varphi}^{c}_{24,j}(-1)^{i} + \sum_{k=1}^{23}\left\{ \bar{\varphi}^{c}_{k,j} \text{ Cos } \frac{2\pi ki}{48} + \bar{\varphi}^{s}_{k,j} \text{ Sin } \frac{2\pi ki}{48} \right\} \qquad (17)$$

where

and

$$\left.\begin{aligned} \bar{\varphi}^{c}_{k,j} &= \frac{2}{48}\sum_{i=0}^{47}\varphi_{i,\,j} \textbf{ cos } \frac{2\pi ki}{48} \\ \bar{\varphi}^{s}_{k,j} &= \frac{2}{48}\sum_{i=0}^{47}\varphi_{i,j} \text{ Sin } \frac{2\pi ki}{48} \end{aligned}\right\} \qquad (18)$$

with analogous expressions for $q^{*}_{i,j}$, $\bar{q}^{c*}_{k,j}$ and $\bar{q}^{s*}_{k,j}$.

The Sine and Cosine functions satisfy the orthogonality relations

$$\sum_{i=0}^{47} \cos \frac{2nki}{48} \cos \frac{2\pi \ell i}{48} = \delta_{k\ell}\,\frac{48}{2} \qquad k,\ a = 1,\ 2, \ldots \mathbf{23}$$

$$\sum_{i=0} \cos \frac{2nki}{48} \cos \frac{2\pi \ell i}{48} = \delta_{k\ell}\ 48 \qquad \mathbf{k} = \ell = 0 \text{ or } 24$$

$$(19)$$

$$\sum_{i=0}^{47} \text{Sin } \frac{2nki}{48} \text{ Sin } \frac{2\pi \ell i}{48} = \delta_{k\ell}\,\frac{48}{2} \qquad k,\ a = 1,\ 2, \ldots \mathbf{23}$$

$$\sum_{i=0}^{7} \text{Sin } \frac{2nki}{48} \text{ Cos } \frac{2\pi \ell i}{48} = 0 \qquad \begin{aligned} &k = 1,\ 2,\ \ldots,\ \mathbf{23} \\ &\mathbf{a} = 0,\ \mathbf{1},\ \ldots,\ 24 \end{aligned}$$

Substituting the expansion **(17)** into (14) and using the orthogonality relations (19) we get the finite Fourier transform of equation (14)

$$\bar{\varphi}_{k,j-2} + \lambda_{k}\,\bar{\varphi}_{k,j} + \bar{\varphi}_{k,j+2} = \bar{q}^{*}_{k,j} \qquad (20)$$

where $\bar{\varphi}$ and $\bar{q}*$ refer to either the sine or cosine harmonic and

$$\lambda_{k} = -2(8 - \mathbf{8} \text{ Cos } \frac{2\pi k}{48} + \text{Cos } \frac{4\pi k}{48}) \qquad (21)$$

We note that, because the chosen sines and cosines are the eigen functions of the matrix A, the equations (20) are 48 independent sets of 24 equations, one set for each of the **48** harmonic amplitudes.

The fourier transform of the modified charge distribution on the even lines, $\bar{q}^*_{k,j}$, may overwrite the modified charge density on these lines. The storage layout and resulting interaction module is shown in FIG lc.

6. Recursive cyclic reduction.

The set of 24 equations for any of the 48 harmonic amplitudes may be written

$$\varphi_{j-2} + \lambda \varphi_j + \varphi_{j+2} = q_j \qquad (22)$$

$$j = 0, 2, \ldots, 46$$

where the bar, star and constant subscript k have been dropped for brevity. These equations form a tridiagonal system with periodic boundary conditions and a particularly efficient method of solution has been devised in collaboration with Dr. G. Golub. This involves the recursive application of the process of cyclic reduction as follows.

Equation (22) is identical in form to equation (10) except that the matrix A is replaced by the scalar λ and the subscript advances in steps of 2 instead of 1.

The process of reducing the number of equations by half as described in equations (13) and (14) may now be similarly applied, leading to 12 equations linking every fourth line, namely:

$$\varphi_{j-2^2} + \lambda^{(2)} \varphi_j + \varphi_{j+2^2} = q_j^{(2)} \qquad (23)$$

$$\mathbf{j = 0, 4, \ldots, 44}$$

where

$$\left.\begin{aligned} \lambda^{(2)} &= 2 - \lambda^2 \\ \text{and} \qquad q_j^{(2)} &= q_{j-2} - \lambda\, q_j + q_{j+2} \end{aligned}\right\} \qquad (24)$$

The 12 equations (23) are of identical form to the equations (22) but with a modified right-hand side, q_j, and central coefficient, λ, as given by equation (24). The quantity $q_j^{(2)}$ may, for storage economy, overwrite the $q_0, q_4, q_8 \;.\;.\;.\; q_{44}$, while $q_2, q_6, q_{10} \;.\;.\;.\; q_{46}$ are kept unchanged in their location.

The process of reduction may therefore be carried out recursively until a small number of equations are obtained which are solved directly.

If we let 't' be the depth of the recursion the recurrence formulae become

$$\varphi_{j-2^t} + \lambda^{(t)} \varphi_j + \varphi_{j+2^t} = q_j^{(t)} \qquad (25)$$

for $j = 0, 2^t, \ldots, (48-2^t)$

$$\left.\begin{aligned} \text{where} \qquad \lambda^{(t+1)} &= 2 - (\lambda^{(t)})^2 \\ q_j^{(t+1)} &= q_{j-2^t}^{(t)} - \lambda^{(t)} q_j^{(t)} + q_{j+2^t}^{(t)} \end{aligned}\right\} \qquad (26)$$

$$\left.\begin{aligned} \text{with} \qquad \lambda^{(1)} &= \lambda \\ q_j^{(1)} &= \overline{q_j^*} \end{aligned}\right. \qquad (27)$$

Three applications of the reduction process leave us with 3 equations for φ_o, φ_{16} and φ_{32} which cannot be further reduced, namely:

$$C\,\underset{\sim}{\varphi} = \begin{pmatrix} \lambda^{(4)} & 1 & 1 \\ 1 & \lambda^{(4)} & 1 \\ 1 & 1 & \lambda^{(4)} \end{pmatrix} \begin{pmatrix} \varphi_o \\ \text{“16} \\ \varphi_{32} \end{pmatrix} = \begin{pmatrix} q_o^{(4)} \\ q_{16}^{(4)} \\ q_{32}^{(4)} \end{pmatrix} = \underset{\sim}{q} \qquad (28)$$

The eigen-values, μ_i, and vectors, u_1 of the matrix C are known:

$$\left.\begin{array}{lll} \underset{\sim}{u}_1' = (1, 1, 1,) & \text{with} & \mu_1 = 2 + \lambda^{(4)} \\ \underset{\sim}{u}_2' = (1, -2, 1) & & \mu_2 = \lambda^{(4)} - 1 \\ \underset{\sim}{u}_3' = (1, 0, -1) & & \mu_3 = \lambda^{(4)} - 1 \end{array}\right\} \qquad (29)$$

where the prime denotes transpose.

Expanding the solution in terms of the eigen-vectors.

$$\underset{\sim}{\varphi} = \alpha_1\, \underset{\sim}{u}_1 + \alpha_2\, \underset{\sim}{u}_2 + \alpha_3\, u_3 \qquad (30)$$

then

$$C\underset{\sim}{\varphi} = \underset{\sim}{q} = \alpha_1\, \mu_1\, u_1 + \alpha_2\, \mu_2\, u_2 + \alpha_3\, \mu_3\, u_3 \qquad (31)$$

and

$$\left.\begin{array}{l} \alpha_1 = \dfrac{\underset{\sim}{u}_1' \cdot \underset{\sim}{q}}{u_1' \cdot u_1} = \dfrac{q_o^{(4)} + q_{16}^{(4)} + q_{32}^{(4)}}{3(\lambda^{(4)} + 2)} \\[2ex] \alpha_2 = \dfrac{\underset{\sim}{u}_2' \cdot \underset{\sim}{q}}{u_2' \cdot u_2} = \dfrac{q_o^{(4)} - 2q_{16}^{(4)} + q_{32}^{(4)}}{6(\lambda^{(4)} - 1)} \\[2ex] \alpha_3 = \dfrac{\underset{\sim}{u}_3' \cdot \underset{\sim}{q}}{u_3' \cdot u_3} = \dfrac{q_o^{(4)} - q_{32}^{(4)}}{2(\lambda^{(4)} - 1)} \end{array}\right\} \qquad (32)$$

substituting equations (32) into (30) we get the solution

$$\left.\begin{array}{l} \varphi_o = \alpha_1 + \alpha_2 + a_3 \\ \varphi_{16} = \alpha_1 - 2\alpha_2 + a_3 \\ \varphi_{32} = \alpha_1 - \alpha_3 \end{array}\right\} \qquad (33)$$

In order to find the other values of φ we interpolate intermediate values recursively. First determining $\varphi_8, \varphi_{24}, \varphi_{40}$ then $\varphi_4, \varphi_{12}, \varphi_{20}, \varphi_{28}, \varphi_{36}, \varphi_{44}$, etc. from the relation

$$\varphi_j = \frac{1}{\lambda^{(t)}} \left\{ q_j^{(t)} - \varphi_{j-2^t} - \varphi_{j+2^t} \right\} \qquad (34)$$

for $t = 3, 2, 1$ and for $j = 2^t$ step 2^{t+1} until $(48 - 2^t)$ where all the quantities on the right hand side are known.

The process of cyclic reduction described here is essentially a floating point algorithm due to the fact that the magnitude of $\lambda^{(t)}$ can grow very quickly particularly for the higher harmonics. Consider for example the harmonic with k = 24, when

$$\left.\begin{aligned} \lambda_{24}^{(1)} &= -34 \\ \lambda_{24}^{(2)} &= -1154 \\ \lambda_{24}^{(3)} &= -1.33 \times 10^{6} \\ \lambda_{24}^{(4)} &= -1.77 \times 10^{12} \end{aligned}\right\} \qquad (35)$$

This might be thought of as a disadvantage, bringing as it does the danger of machine overflow. In fact the phenomonon may be turned to advantage on a floating point machine-by noticing that if, at any level of the reduction, $\lambda^{(t)} > 10^n$ and we are only interested in computing with a precision of 1 part in 10^n, then equation (25) may be written

$$\lambda^{(t)} \varphi_j = q_j^{(t)} \qquad (36)$$

for $j = 0$ step 2^t until $(48 - 2^t)$

where the first and third terms of the left hand side have been neglected in comparison with the second.

Thus the solution φ_j at the t^{th} level can be determined by simple division from equation (37)

$$\varphi_j = \frac{q_j^{(t)}}{\lambda^{(t)}} \qquad (37)$$

and interpolation of intermediate values started immediately.

An alternative scaling of the cyclic reduction method can be made in which numbers decrease in magnitude and which is therefore suitable for a fixed point machine. However it appears that an extra multiplication is introduced.

7. Solution on the Even lines.

The solution of the equations (22) by the technique of recursive cyclic reduction has determined the values of all 48 harmonic amplitudes on the 24 'even' lines of the mesh. The solution on the even lines is found by the process of Fourier synthesis using equation (17), and the stage indicated by FIG 1d is reached.

8. Solution on the Odd lines.

The solution for the potential on the odd lines can be found from equation (13).

$$A\,\underset{\sim}{\varphi}_j = \underset{\sim}{q}_j - \underset{\sim}{\varphi}_{j-1} - \underset{\sim}{\varphi}_{j+1} \qquad (38)$$

for j = 1 step 2 until 47

where the potential vectors on the right hand side are the known values on the even lines.

The equation (38) is a tridiagonal system with periodic boundary conditions and again is most conveniently solved by recursive cyclic reduction, starting from the expanded form of equation (38)

$$\varphi_{i+1,j} - 4 \quad , \varphi_{i} \quad \varphi_{,i+1} = {}_{,}q_{i} - \varphi_{,i\ j-1} - \varphi_{i,j+1} \qquad (39)$$

for j = 1 step 2 until **47**, for i = 0 step 1 until **47**

9. Operation Count and Speed

In order to get more general formulae for the number of operations we shall consider an $(n \times m)$ mesh where the Fourier analysis is performed in the 'n' direction. The number of operations for the different stages of the calculation are as follows:

a) Form modified charge density on even lines,

According to equation **(16)** this takes **5** additions per point*. There are n points per line and m/2 lines therefore a total of

$$\left.\begin{array}{l} n \times \frac{m}{2} \times 5 = 2\tfrac{1}{2}\ nm \text{ additions} \\ \text{and zero multiplications} \end{array}\right\} \qquad (40)$$

b) Fourier analysis of the modified charge on even lines,

According to equation **(18)** Fourier analysis would require n multiplications and n additions per harmonic per line, There are n harmonics and m/2 lines therefore without any simplification we get a total of

$$\left.\begin{array}{l} n \times n \times \frac{m}{2} = \frac{n^2}{2}\, m \text{ additions} \\ \text{and} \qquad \frac{n^2}{2}\, m \text{ multiplications} \end{array}\right\} \qquad (41)$$

If however we make use of the symmetry of the sines and cosines, grouping and adding together all terms multiplied by the same factor, before performing the multiplication, the number of operations can be drastically reduced, See for example Whittaker and Robinson [3].

*The multiplication by 4 is an addition to the exponent of a floating point number.

For the case n = 48 which has been programmed we find that all 48 harmonics on a given line can be found with 325 additions and 89 multiplications. For this spot case of n = 48 this corresponds to $\frac{n^2}{7}$ additions and $\frac{n^2}{26}$ multiplications to determine all the harmonics on one line, giving a total with grouping of

$$\left.\begin{array}{l} \frac{m}{2} \times \frac{n^2}{7} = \frac{n^2}{14}\, m \text{ additions} \\ \frac{m}{2} \times \frac{n^2}{26} = \frac{n^2}{52}\, m \text{ multiplications} \end{array}\right\} \qquad (42)$$

c) <u>Solution of harmonic amplitudes of potential on even lines.</u>

For a line of points 48 long equations (27) and (34) show the operational counts for the process of cyclic reduction to be

2 × 24 additions and 24 multiplications to find $q^{(2)}$ from $q^{(1)}$

2 x 12 additions and 12 multiplications to find $q^{(3)}$ from $q^{(2)}$

2 × 6 additions and 6 multiplications to find $q^{(4)}$ from $q^{(3)}$

8 additions and 7 multiplications to find $\varphi_o, \varphi_{16}, \varphi_{32}$

2 × 3 additions and 3 multiplications to find $\varphi_8, \varphi_{24}, \varphi_{40}$

2 × 6 additions and 6 multiplications to find $\varphi_4, \varphi_{12}, \dots, \varphi_{44}$

2 × 12 additions and 12 multiplications to find $\varphi_2, \varphi_6, \dots, \varphi_{46}$

2 × 24 additions and 24 multiplications to find $\varphi_1, \varphi_3, \dots \varphi_{47}$

2 × 95 additions and 94 multiplications in total

In general we may say for a line q points long cyclic reduction takes

4 × q additions and 2 × q multiplications (43)

In the determination of the harmonic amplitudes at this stage there are n tridiagonal systems to be solved each $\frac{m}{2}$ long. The total count is

$$\left.\begin{array}{ll}\text{therefore} & 4 \times n \times \frac{m}{2} = 2\ n\ m \text{ additions} \\ \text{and} & 2 \times n \times \frac{m}{2} = \ \ n\ m \text{ multiplications}\end{array}\right\} \quad (44)$$

d) Fourier synthesis.

The Fourier synthesis required to obtain the potential from the harmonic amplitudes of potential via equation (17) can be simplified by grouping of terms to the same number of operations as for Fourier analysis in step b) giving a further

$$\left.\begin{array}{ll} & \frac{n^2}{14} m \text{ additions} \\ \text{and} & \frac{n^2}{52} m \text{ multiplications}\end{array}\right\} \quad (45)$$

e) Solution on Odd lines.

First we form the right hand side of equation (38) for all points on the odd lines. There are $n \times \frac{m}{2}$ such points giving $2 \times \frac{nm}{2} = nm$ additions,

Next the tridiagonal system of equation (38) is solved by recursive cyclic reduction. There are $\frac{m}{2}$ such systems each n equation long, Using the results of c) we have for the solution of these equations

$$\left.\begin{array}{ll} & 4 \cdot n \cdot \frac{m}{2} = 2\ n\ m \text{ additions} \\ \text{and} & 2 \cdot n \cdot \frac{m}{2} = \ \ n\ m \text{ multiplications}\end{array}\right\} \quad (46)$$

The total operations for stage e) is therefore

$$\left.\begin{array}{ll} & 3\ n\ m \text{ additions} \\ \text{and} & n\ m \text{ multiplications}\end{array}\right\} \quad (47)$$

Total operations and storage,

The number of operations for the solution of Poisson's equation given a right-hand side is therefore

$$\begin{gathered}(\frac{n^2m}{7} + 7\,\frac{1}{2}\;n\;m)\text{ additions and }(\frac{n^2m}{26} + 2\;n\;m)\text{ multiplications} \\ \text{or in total }(\frac{n^2m}{5.5} + 9\,\frac{1}{2}\;n\;m)\text{ arithmetic operations}\end{gathered} \qquad (48)$$

where it must be remembered that the reduction factors of 7 and 26 appearing in the n^2 terms are known to be true only if n = 48. In general these reduction factor may well be functions of n.

Throughout the process new results may overwrite old and we need basically only one mesh of (n × m) storage locations, These originally contain the charge distribution which is overwritten by the Fourier transform of the charge, which is overwritten by the Fourier transform of the potential, which is finally overwritten by the potential solution.

The only other storage required is for the Fourier harmonics themselves. In general there would be (n × n) numbers describing the shape of the n harmonics however due to the symmetry of the sines and cosines only $\frac{n}{4}$ distinct numbers occur.

The total date storage is therefore $(n \times m + \frac{n}{4})$.

Tables 2 and 3 show the estimated times for each stage in the process using the operation counts above for the IBM 7090 and 7094, together with the measured time on the 7090.

For the purpose of estimation we have used the following speeds for the floating point operations

Machine	addition	multiplication
IBM 7090	15μs	25μs
IBM 7094	6μs	10μs

TABLE 1.

The measured time is taken from a floating point symbolic FAP program, Due to the large number of additions some increased in speed could be obtained by programming in fixed point.

IBM 7090

Stage	additions	estimated time secs	mults	estimated time secs	Total estimated time	measured time
a	2 1/2 n	m 00086	0	0	00086	0.319
b	$\frac{n^2m}{14}$	0.118	$\frac{n^2m}{5\ 2}$	0.053	0.171	
c	2nm	0.069	n m	0.058	0.127	0.168
d	$\frac{n^2m}{14}$	00118	$\frac{n^2m}{5\ 2}$	0.058	**00171**	0.230
e	3 n m	**0.103**	n m	0.058	0.161	0.189
Solution of Poissons equation on **48** × 48 mesh					= **0.716**	0.906

TABLE 2.

IBM 7094

Stage	additions	estimated time	mults	estimated time	Total estimated time	time
a	2 1/2 n m	0.035	0	0	0.035	
b	$\frac{n^2m}{14}$	0.047	$\frac{n^2m}{52}$	0,021	0.068	
c	2 n m	0.028	n m	0.023	0.051	
d	$\frac{n^2m}{14}$	0.047	$\frac{n^2m}{52}$	00021	00068	
e	3 n m	0.041	n m	0.023	0.064	
Solution of Poissons equation on 48 x 48 mesh					= 0.286	0.358

TABLE 3.

The difference between the measured and estimated times of about 25% is accounted for by computer 'housekeeping' operations. Using this factor on the 7094 estimated figure we obtain 0.358 secs as a realistic estimate for the time of solution on the 7094. It is interesting to note from Table 2 that two frequently repeated generalizations are untrue. It is not even approximately true, for example, that additions may be neglected compared with multiplications, because in each stage of the process the time spent on additions is in fact greater than the time spend on multiplications. It is also untrue that it is satisfactory to consider only the highest power of 'n' for in this case the time spend computing the stages with operations proportional to n^2m is less than the time spent on stages with operations proportional to n m.

10. Accuracy

The accuracy of the method has been examined by testing its ability to reproduce a given random distribution of potential.

We start by generating a random distribution of potential, φ^*, on the points of the mesh. Next the charge distribution, q, which corresponds exactly to φ^* is computed from equation (8) namely

$$q_{i,j} = \varphi^*_{i-1,j} + \varphi^*_{i+1,j} + \varphi^*_{i,j-1} + \varphi^*_{i,j+1} - 4\,\varphi^*_{i,j} \qquad (50)$$

The Fourier technique was then used to derive a potential distribution, φ, from the charge distribution q_{ij}, and the exact distribution φ^* and the solution φ were examined,

The random distribution generated varied between -1/2 and +1/2 and the largest value of the error, $(\varphi^* - \varphi)$, obtained with 7 different distributions was 3.3×10^{-7}.

11. Generalization

11.1 Solution of matrix equations

Consider the general matrix equations

$$B\,\underset{\sim}{\varphi} = \underset{\sim}{q} \qquad (51)$$

where B is partitioned into (m × m) square blocks B_{ij} of size (n x n). $\underset{\sim}{\varphi}$ are $\underset{\sim}{q}$ are partitioned into (m × 1) vectors $\underset{\sim}{\varphi}_j$ of length (n × 1).

$$B = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1m} \\ B_{21} & B_{22} & & \\ \vdots & & \ddots & \\ B_{m1} & & & B_{mm} \end{pmatrix}, \quad \underset{\sim}{\varphi} = \begin{pmatrix} \underset{\sim}{\varphi}_1 \\ \underset{\sim}{\varphi}_2 \\ \vdots \\ \underset{\sim}{\varphi}_m \end{pmatrix}, \quad \underset{\sim}{q} = \begin{pmatrix} \underset{\sim}{q}_1 \\ \underset{\sim}{q}_2 \\ \vdots \\ \underset{\sim}{q}_m \end{pmatrix} \qquad (52)$$

Such a system of partitioned equations naturally arises in the finite difference form of a two-dimensional partial differential equations, when the mesh is confined to a -rectangular region with m lines each containing n mesh points.

The Fourier technique can be applied to the solution of equation (51) provided each block matrix B_{ij} can be diagonalised by the same similarity transformation.

If this is the case let the $(n \times n)$ transformation matrix be Q and the resulting $(n \times n)$ diagonal matrices be D_{ij}

then
$$Q^{-1} B_{ij} Q = D_{ij} \tag{53}$$

We can also define the transformed vectors

$$\left.\begin{aligned} \bar{\underset{\sim}{\varphi}}_j &= Q^{-1} \underset{\sim}{\varphi}_j \\ \text{and} \qquad \bar{\underset{\sim}{q}}_j &= Q^{-1} \underset{\sim}{q}_j \end{aligned}\right\} \tag{54}$$

with the inverse transformation

$$\left.\begin{aligned} \underset{\sim}{\varphi}_j &= Q \bar{\underset{\sim}{\varphi}}_j \\ \text{and} \qquad \underset{\sim}{q}_j &= Q \bar{\underset{\sim}{q}}_j \end{aligned}\right\} \tag{55}$$

where

$$\underset{\sim}{\varphi}_j = \begin{pmatrix} \varphi_{1j} \\ \varphi_{2j} \\ \circ \\ \circ \\ \circ \\ \varphi_{nj} \end{pmatrix} \qquad \bar{\underset{\sim}{\varphi}}_j = \begin{pmatrix} \bar{\varphi}^1_j \\ \bar{\varphi}^2_j \\ \circ \\ \circ \\ \circ \\ \bar{\varphi}^n_j \end{pmatrix} \tag{56}$$

and j = 1 step 1 until m.

The operation Q^{-1} can be seen to correspond to the step of Fourier analysis and Q to Fourier synthesis in the example given earlier in this paper. In general we shall refer to the operation Q^{-1} on the vector $\underset{\sim}{\varphi}_j$ as the analysis of the vector into harmonic components $\bar{\varphi}_j^k$ and the operation Q is the synthesis of the harmonic components $\bar{\varphi}_j^k$ into the actual vector components $\varphi_{i,j}$ of $\underset{\sim}{\varphi}_j$. This process becomes Fourier analysis and synthesis in the special case that the vectors comprising the transformation matrix Q are sines and cosines.

Consider the i^{th} row of equation (51)

$$\left.\begin{aligned} \sum_{j=1}^{m} B_{ij} \underset{\sim}{\varphi}_j &= \underset{\sim}{q}_i \\ \sum_{j=1}^{m} B_{ij}\, Q\, \underset{\sim}{\bar{\varphi}}_j &= Q\, \underset{\sim}{\bar{q}}_i \end{aligned}\right\} \qquad (57)$$

multiplying through by Q^{-1} we have

$$\sum_{j=1}^{m} Q^{-1} B_{ij}\, Q\, \underset{\sim}{\bar{\varphi}}_j = \underset{\sim}{\bar{q}}_i$$

or

$$\sum_{j=1}^{m} D_{ij}\, \underset{\sim}{\bar{\varphi}}_j = \underset{\sim}{\bar{q}}_i \qquad (58)$$

writing equation (58) in full and writing the diagonal elements of D_{ij} as $\bar{D}_{ij}^k$ we have:

$$\sum_{j=1}^{m} \begin{pmatrix} \bar{D}_{ij}^1 & & & 0 \\ & \bar{D}_{ij}^2 & & \\ & & \cdot & \\ 0 & & & \cdot \; \bar{D}_{ij}^n \end{pmatrix} \begin{pmatrix} \bar{\varphi}_j^1 \\ \bar{\varphi}_j^2 \\ \vdots \\ \bar{\varphi}_j^n \end{pmatrix} = \begin{pmatrix} \bar{q}_i^1 \\ \bar{q}_i^2 \\ \vdots \\ \bar{q}_i^n \end{pmatrix} \qquad (59)$$

for i = 1 step 1 until m.

The equations for different harmonic numbers are independent and the equations (59) may be reordered to give n independent sets of m equations, one set for each of the harmonic numbers.

$$\begin{pmatrix} \bar{D}^k_{11} & \bar{D}^k_{12} & \cdots & \bar{D}^k_{1m} \\ \bar{D}^k_{21} & \bar{D}^k_{22} & \cdots & \bar{D}^k_{2m} \\ \vdots & & & \\ \bar{D}^k_{n1} & \cdots & \cdots & \bar{D}^k_{mm} \end{pmatrix} \begin{pmatrix} \bar{\varphi}^k_1 \\ \bar{\varphi}^k_2 \\ \vdots \\ \bar{\varphi}^k_m \end{pmatrix} = \begin{pmatrix} \bar{q}^k_1 \\ \bar{q}^k_2 \\ \vdots \\ \bar{q}^k_m \end{pmatrix} \qquad (60)$$

for k= 1 step 1 until n.

The Fourier technique of solution of the equations (51) would proceed as follows:

a) analyse each line into harmonics by the operation Q^{-1} as in equation (54). In the absence of any symmetry in the matrix Q this leads to

n^2m additions

and n^2m multiplications

b) Solution of the sets of equations (60) for each harmonic number. Solution by a direct method would require of the order m^3 multiplications per harmonic or a total of

$n\ m^3$ multiplications

c) Synthesis on each line by the operation Q as in equation (55). As in step a) this leads at worst to

n^2m additions

and n^2m multiplications

In total the set of n × m equations (51) can be solvedbythe Fourier method with about $n\ m^3 + 2\ n^2 m$ operations. A direct method such as gauss elimination applied directly to (51) would require of the order $(n\ m)^3 = n^3 m^3$ operations.

A Block Gauss-Seidel iteration on equation (51) would require the order of $n^2 m$ operations per iteration. The iterative method would be faster if the number of iterations required was less than 'm', which is a plausible situation.

The Fourier method is much more likely to be faster for problems in which the transformation matrix Q and Q^{-1} have symmetry, so that the number of operations required in forming the product $Q^{-1}q$ in step a) and $Q\ \varphi$ in step c) can be reduced to $\frac{n^3}{F}$, where F is some factor of reduction. In the special case discussed earlier when Sines and Cosines are the components of Q, F is about 10.

The Fourier method will benefit further if special direct methods are available for the solution of equation (60) in step b). In the case that the matrix operator in equation (60) can be diagonalised by the same similarity transformation for every value of k then equation (60) can itself be solved by the Fourier technique. This would require of the worst of the order $n(m^2 + m\}$ instead of $n\ m^3$. Also if (60) is tridiagonal then (60) may be solved in the order of m operations for every k or a total of the order n m operations. Furthermore if the Block form of the matrix B is tridiagonal it is likely to be worthwhile to perform at least one step of Odd/Even reduction before introducing harmonic analysis, as described earlier in section 4.

11.2 Solution of Differential equations

An important class of differential equations which lead to matrices of the form that can be solved by the Fourier method are those of the form

$$\{ L(x) + M(y) \} \varphi(x,y) = s(x,y) \qquad (61)$$

where L(x) is a linear operator which may be a function of x only and M(y) a function of y only. The boundary conditions must be specified on the surface of the rectangle, $0 < x \leq \ell_1$, $0 < y \leq \ell_2$ and be of the form

$$\left.\begin{aligned} a_1 \frac{\partial\varphi}{\partial x} + b_1 \varphi &= c_1(y) \text{ along } x = 0 \\ a_2 \frac{\partial\varphi}{\partial x} + b_2 \varphi &= c_2(y) \text{ along } x = \ell_1 \end{aligned}\right\} \qquad (62)$$

or the periodic condition $\varphi(x,y) = \varphi(x + \ell_1, y)$ where a_1, a_2, $b_{1'}$ b_2 are constants c_1, c_2 may be functions of y and the form

$$\left.\begin{aligned} a_3(x) \frac{\partial\varphi}{\partial y} + b_3(x) \varphi &= c_3(x) \text{ along } y = 0 \\ a_4(x) \frac{\partial\varphi}{\partial y} + b_4(x) \varphi &= c_4(x) \text{ along } y = \ell_2 \end{aligned}\right\} \qquad (63)$$

or the periodic condition $\varphi(x,y) = \varphi(x,y + \ell_2)$ where all a, b, c may depend on x.

Examples of equations satisfying these conditions are Laplaces, Poissons, and Helmhotz equation in a rectangle where all parameters occuring in the equation and boundary conditions are either constant, or depend on only one variable. The coordinate system may be any pair of coordinates from Cartesian, polar, or spherical systems.

These are

$$\nabla^2 \varphi = 0$$

$$\nabla^2 \varphi = \rho$$

$$\nabla^2 \varphi + k^2 \varphi = s$$

It is interesting to note that in the case of Laplace's equation there is no change in the complexity of the calculation if the nine point finite difference module is used instead of the more common five point formula.

The biharmonic equation, $\nabla^4 \varphi = 0$, in the rectangle may also be solved with the 25 point difference module [4].

If the index, i, corresponds to the variable x and, j, to the variable y then the finite difference form of equation (61) will be

$$\{ L_i + M_j \} \varphi_{ij} = s_{ij} \qquad (64)$$

where L_i and M_j are difference operators acting on the indices i and j respectively. Any finite difference mesh may be taken within the rectangle and we suppose $i = 1, 2, \ldots . n$ and $j = 1, 2, \ldots) m$.

The matrix form of equation (64) is of the form of equation (51) with B_{ij} a multiple of the identity matrix if $i \neq j$. The restricted form of boundary'conditions (62) ensures that $B_{11} = B_{22} = \cdots = B_{mm}$ and the condition is satisfied that all B_{ij} can be diagonalized by the same similarity transformation. The transformation matrix Q is the matrix formed by all the eigenvectors of B_{11} which can be precalculated.

If the boundary conditions at y = 0, ℓ_2 are also of the restricted kind of equation (62) then x and y can be interchanged and the transformation matrix can be formed from the eigenvectors of the matrix equivalent of the operator M_J. Which choice is the better depends on a balance between the symmetry of the eigenvectors and the length of the eigenvector. The greater the symmetry the larger will be the reduction factor F in the analysis and synthesis steps. On the other hand the number of operations is $\frac{n^2m}{F}$ and increases rapidly with the length of the vector, that is to say the number of mesh points in the direction of the analysis. To increase the value of F it will be advantageous to have a uniform mesh spacing in the direction of the harmonic analysis.

If we are concerned with second order equations it appears that the greatest amount of symmetry in the matrix Q occurs if its component eigenvectors are sines and cosines which have zero slope or value or are periodic at the boundaries. This implies that the operator in the chosen direction of analysis is simply $\{ \frac{d^2}{dx^2} + k^2 \}$ and the boundary conditions (62) are further restricted to be of the form

$$\left.\begin{array}{l} \text{either } \frac{\partial\varphi}{\partial x} = 0 \text{ or } \varphi = 0 \text{ along } x = 0 \\ \text{either } \frac{\partial\varphi}{\partial x} = 0 \text{ or } \varphi = 0 \text{ along } x = \ell_1 \end{array}\right\} \quad (65)$$

or the periodic condition $\varphi(x,y) = \varphi(x + \ell_1,y)$.

In certain cases it may be worthwhile performing a transformation on the whole problem to achieve this simple form. FIG 2 shows diagramatically the types of problems most suitable for solution by the Fourier method.

The Fourier method, providing as it does a fast method for the solution of Poissons equation over a rectangle, can be used as the basis for various block iterative schemes for more complex regions that can be divided up into rectangles. One could consider for example a block 48-line iteration analogous to the block l-line and 2-line methods [5].

Conclusion

For the special problems involving (x,y) geometry in the rectangle for which the Fourier method is well suited there seems little doubt that it is a faster method of calculation than any direct or iterative method so far suggested.

For other problems where the method can be applied but is not well suited the position is less clear and we will have to await the results of practical numerical experiments before the fastest method can be chosen.

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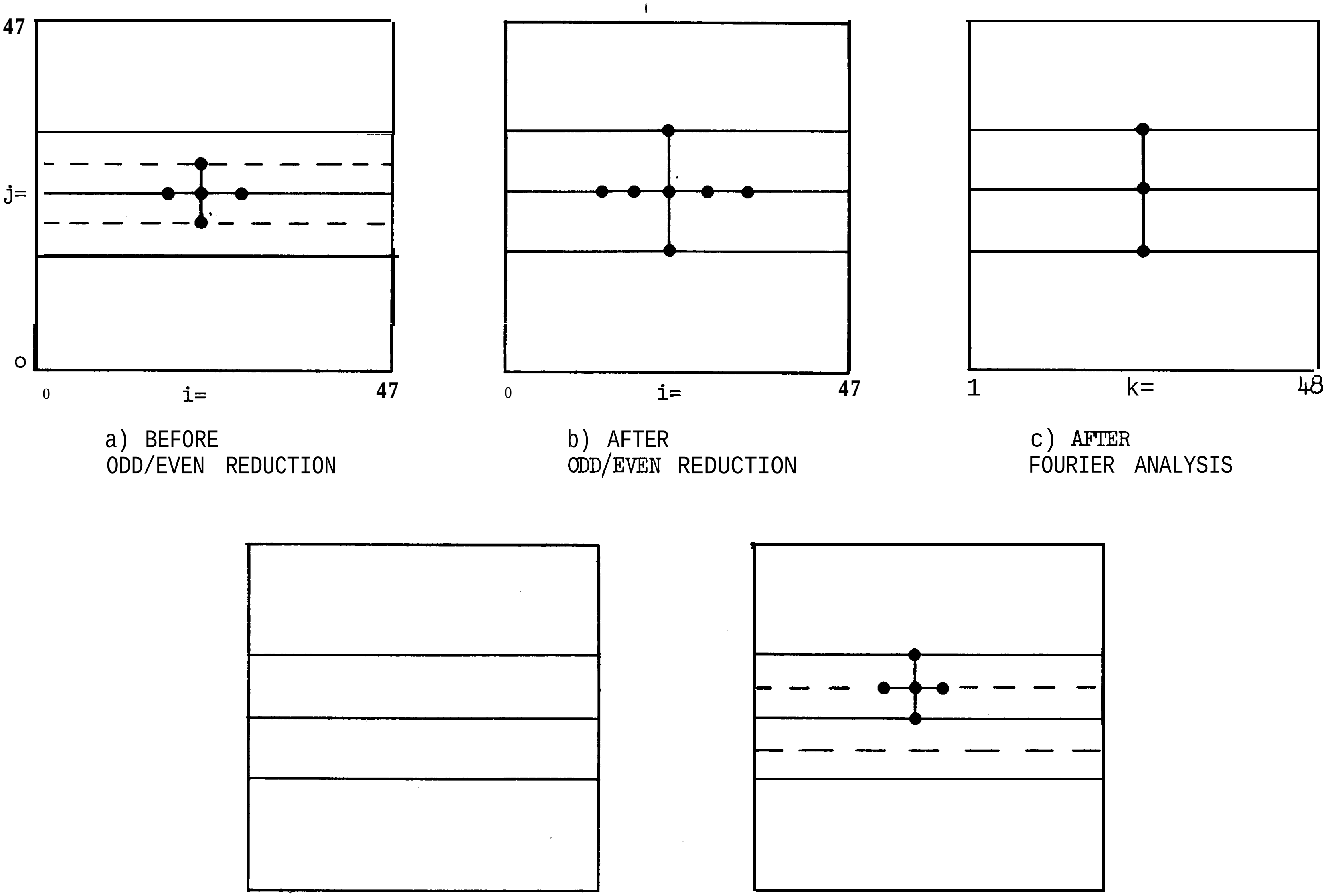

a) BEFORE
ODD/EVEN REDUCTION

b) AFTER
ODD/EVEN REDUCTION

c) AFTER
FOURIER ANALYSIS

d) AFTER
FOURIER SYNTHESIS

e) SOLUTION ON
ODD LINES

FIG 1

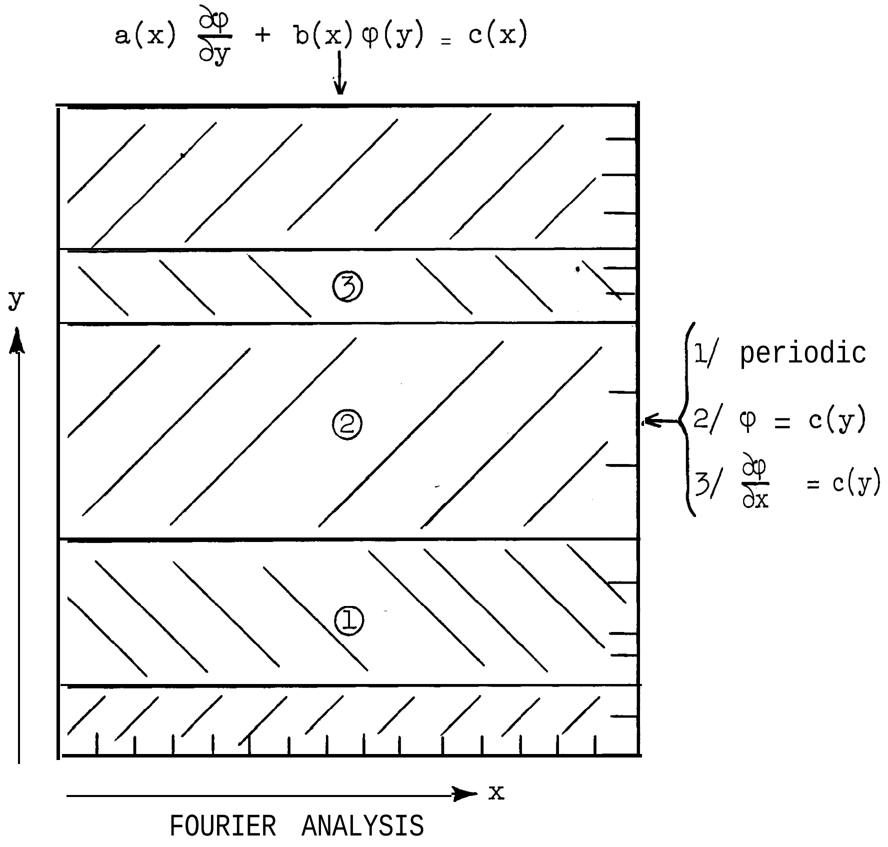
$a(x)\frac{\partial\varphi}{\partial y} + b(x)\varphi(y) = c(x)$
y
③
②
①
1/ periodic
2/ $\varphi = c(y)$
3/ $\frac{\partial\varphi}{\partial x} = c(y)$
x
FOURIER ANALYSIS

FIG 2

PROBLEMS MOST SUITABLE FOR FOURIER METHOD

a) Rectangular region

b) slab type property changes ①, ② etc.

c) simple boundary conditions

d) uniform mesh at least in analysis direction

e) typical equation

$$\nabla D(y)\,\nabla\varphi(x,y) + k^2(y)\,\varphi(x,y) = S(x,y)$$