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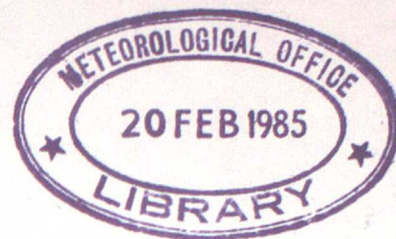
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MET.O.15 INTERNAL REPORT

58

A DIRECT POISSON SOLVER WITH
NEUMANN BOUNDARY CONDITIONS ON A
STAGGERED GRID

BY

C.S. VAN DEN BERGHE

1. INTRODUCTION

This note describes the method of solution adopted for the solution of a three dimensional Poisson equation. The equation arises from the solution of the three dimensional anelastic equations. The methods used (Fourier transform and Gaussian elimination) are conventional and well described in the open literature. However it is felt that the particular problem solved is unique enough (Neumann boundary conditions with a staggered grid) for the algorithm to be described in detail. The purposes of this note are thus to document the subroutine produced, to provide a full description of a Poisson solver algorithm and to correct errors in a description of the Fourier Transform algorithm given by Wilhelmson and Ericksen (1977).

The next section defines the problem and is followed by a detailed description of the algorithm; the final section documents the main subroutine that has been coded.

For efficiency of calculation the subroutine has not been written in an entirely general form, though modification to related problems should be straightforward.

2. THE PROBLEM

In a three dimensional model using the anelastic equations the perturbation pressure is diagnosed at each time step from a Poisson equation that has the general form (eg Clark (1977) or van den Berghe (1985)).

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] p + \frac{\partial}{\partial z} f(z) p = s \quad [1]$$

where $p(x,y,z,t)$ is the perturbation pressure, $s(x,y,x,t)$ a source term and $f(z)$ is constant in time.

Since the model is of limited lateral extent the boundary conditions at all six boundaries are derived from the momentum equations and take the form of Neumann conditions (Clark (1977)). It is intended to also allow the possibility of an upper boundary condition that (approximately) radiates gravity waves. This condition (Klemp and Durran (1982)) results in a Dirichlet boundary condition for the upper boundary pressure.

Equation 1 is approximated using the finite difference approximation of Piacsek and Williams (1970) on a staggered grid (the Arakawa 'C' grid, see Haltiner and Williams (1980) p226 or van den Berghe (1985)) with all the boundaries passing through momentum (not pressure) points.

An explicit description of our approximation to the above problem follows.

Equation [1] becomes

$$\begin{aligned} \frac{1}{\Delta x^2} \{ P_{i+1} - 2P + P_{i-1} \} + \frac{1}{\Delta y^2} \{ P_{j+1} - 2P + P_{j-1} \} \\ + \frac{1}{DZ} \left\{ \frac{1}{DZN_{k+1}} (P_{k+1} - P) - \frac{1}{DZN} (P - P_{k-1}) \right\} \\ + \frac{1}{2DZ} \{ f_{k+1} - f_{k-1} \} = S \quad [2] \end{aligned}$$

where for clarity the subscripts are only given when they are not equal to (i,j,k). The vertical spacing is assumed to vary and $DZ = z - z_{k-1}$.

$DZN = z_n - z_{n_{k-1}}$ where z is a vertical velocity point and z_n a pressure point. f is assumed to be defined on z points. The physical position of a p point is $((i-1/2)\Delta x, (j-1/2)\Delta y, z_n(k))$, $i=1,2,\dots,II$, $j=1,\dots, JJ$, $k=2,\dots, KK-1$. The boundaries are at $x=0, L_x$, $y=0, L_y$, $z=0, H$ and computational points are assumed at $i=0$ and $II+1$, $j=0$ and $JJ+1$, $k=1$ and KK . Thus $L_x = (II-1)\Delta x$, $L_y = (JJ-1)\Delta y$, $H = z(KK-1) - z(1)$

The boundary conditions are

$$\frac{\partial P}{\partial x} \Big|_{x=0} = \frac{1}{\Delta x} \{ P_{1jk} - P_{0jk} \} = g(0, j, k)$$

$$\frac{\partial P}{\partial x} \Big|_{x=L_x} = \frac{1}{\Delta x} \{ P_{II+1jk} - P_{IIjk} \} = g(L_x, j, k)$$

$$\frac{\partial P}{\partial y} \Big|_{y=0} = g(i, 0, k), \quad \frac{\partial P}{\partial y} \Big|_{y=L_y} = g(i, L_y, k)$$

$$\left[\frac{\partial p}{\partial z} + \frac{g}{\rho} \rho \right]_{z=0} = g(i, j, 0)$$

[3]

$$\left[\frac{\partial p}{\partial z} + \frac{g}{\rho} \rho \right]_{z=H} = g(i, j, H)$$

$$\underline{\text{or}} \quad p_{ijkk} = h(x, y)$$

where $g(x, y, z)$ is the boundary forcing term, derived from the momentum equations.

3. METHOD OF SOLUTION

The most efficient direct solution of the above system is to decouple the equations by using a Fourier transform in two directions and then to solve the decoupled equations by using a direct tridiagonal solver (Wilhelmson and Ericksen (1977)). Noting the structure of equation [2] in the vertical and the possible choices of upper boundary conditions we choose to Fourier transform in the horizontal (x and y) and to use a recursive formula to invert the equations in the vertical. The efficiency of this method can be improved by (a) performing some levels of cyclic reduction between the horizontal transforms, (b) using cyclic reduction or recursive doubling in the vertical. Both methods are vectorizable on the CYBER 205 but it was felt that the extra coding complexity did not warrant this approach since the poisson solver takes only 5% of the model's computer time.

The algorithm can be split into four parts

- (i) basic Fourier transform method
- (ii) manipulation of the Fast Fourier transforms
- (iii) inhomogeneity of problem
- (iv) vertical inversion

The subsections below deal with these aspects in turn.

3(i) To explain the Fourier transform algorithm consider a one dimensional system

$$\frac{1}{\Delta x^2} (p_{i+1} - 2p_i + p_{i-1}) = s_i \quad [4]$$
$$i = 1, 2, \dots, II$$

subject to

$$P_1 - P_0 = 0, \quad P_{II+1} - P_{II} = 0$$

If the pressure and source terms are expanded as

$$P_i = \sum_{\bar{i}=1}^{\Pi} \hat{P}_{\bar{i}} \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-1/2)\right)$$

$$S_i = \sum_{\bar{i}=1}^{\Pi} \hat{S}_{\bar{i}} \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-1/2)\right) \quad [5]$$

equation [4] becomes

$$\frac{1}{\Delta x^2} \sum_{\bar{i}=1}^{\Pi} \hat{P}_{\bar{i}} \left[\cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i+1/2)\right) - 2 \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-1/2)\right) + \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-3/2)\right) \right] = \sum_{\bar{i}=1}^{\Pi} \hat{S}_{\bar{i}} \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-1/2)\right) \quad [6]$$

but

$$\left[\cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i+1/2)\right) - 2 \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-1/2)\right) + \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-3/2)\right) \right] = 2 \left\{ \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)\right) - 1 \right\} \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)(i-1/2)\right)$$

and equating terms in \bar{i} in equation [6] we find

$$\hat{P}_{\bar{i}} = \frac{\hat{S}_{\bar{i}}}{\frac{2}{\Delta x^2} \left\{ \cos\left(\frac{\hat{\Pi}}{\Pi} (\bar{i}-1)\right) - 1 \right\}} \quad \bar{i} = 2, \dots, \Pi \quad [7]$$

If $\bar{i} = 1$ then $\cos(\frac{\pi}{2}(\bar{i}-1)) - 1 = 0$ and \hat{p}_1 is undefined. This is the well known indeterminacy of Neumann boundary conditions and can be resolved by an arbitrary specification of \hat{p}_1 which results in P correct to a constant (only gradients of P have dynamical significance). In the full system (equation [2]) the vertical structure (usually) removes the indeterminacy.

Having found $\hat{p}_{\bar{i}}$ through equation [7] the inverse transform is used to find p_i ie

$$\hat{p}_{\bar{i}} = \frac{1}{\Pi} \sum_{i=1}^{\Pi} p_i \cos \left[\frac{\pi}{2} (\bar{i}-1)(i-\frac{1}{2}) \right] [2 - \delta_{i1}]$$

$\delta = \text{Kronecker Delta}$

[8]

3(ii) The Fourier transform procedure is only efficient when implemented using Fast Fourier Transform (FFT) techniques. The only FFT routine available on the CYBER 205 is one for periodic functions with boundaries at P points (Temperton (1982)). This routine can be used for the transforms (equations [5] and [8]) by performing some pre and post manipulation of the data. Algorithms of this sort were initially derived by Cooley, Lewis and Welch (1970) and for our particular case by Wilhelmson and Ericksen (1977). The algorithm given by Wilhelmson and Ericksen contains some errors and we give the correct version here.

The Fourier analysis (equation [5]) is initiated by

$$v_I = 2s_I, \quad v_{II} = 2s_{II} \quad (\text{if } II \text{ is even})$$

$$v_{2i} = s_{2i} + s_{2i+1}$$

$$v_{2i+1} = s_{2i} - s_{2i+1}$$

The v s are then supplied to a Fourier synthesis routine that uses

$$\hat{v}_{\bar{i}} = \frac{1}{2} [v_I + (-1)^{\bar{i}-1} v_{II}] + \sum_{i=1}^{II/2} v_{2i} \cos\left(\frac{2\pi}{II} i (\bar{i}-1)\right) + v_{2i+1} \sin\left(\frac{2\pi}{II} i (\bar{i}-1)\right)$$

\hat{s} is obtained from the postprocessing

$$\hat{s}_I = \hat{v}_I$$

$$\hat{s}_{\bar{i}} = \frac{1}{2} [(a+b) \hat{v}_{II-\bar{i}+2} - (a-b) \hat{v}_{\bar{i}}]$$

where

$$a = \sin\left(\frac{\pi}{2II} (\bar{i}-1)\right)$$

$$b = \cos\left(\frac{\pi}{2II} (\bar{i}-1)\right)$$

The synthesis (equation [8]) is initiated by

$$\hat{w}_I = \hat{p}_I$$

$$\hat{w}_{\bar{i}} = [(a+b) \hat{p}_{II-\bar{i}+2} - (a-b) \hat{p}_{\bar{i}}]$$

The \hat{w} s are supplied to a Fourier analysis routine using

$$\omega_1 = \frac{1}{\Pi} \sum_{\bar{i}=1}^{\Pi} \hat{\omega}_{\bar{i}}$$

$$\omega_{\Pi} = \frac{1}{\Pi} \sum_{\bar{i}=1}^{\Pi} \hat{\omega}_{\bar{i}} (-1)^{\bar{i}-1}$$

$$\omega_{2i} = \frac{1}{\Pi} \sum_{\bar{i}=1}^{\Pi} \hat{\omega}_{\bar{i}} \cos \left[\frac{2\hat{\Pi}}{\Pi} i (\bar{i}-1) \right]$$

$$\omega_{2i+1} = \frac{1}{\Pi} \sum_{\bar{i}=1}^{\Pi} \hat{\omega}_{\bar{i}} \sin \left[\frac{2\hat{\Pi}}{\Pi} i (\bar{i}-1) \right]$$

P is found after the postprocessing

$$P_1 = \frac{1}{2} \omega_1, \quad P_{\Pi} = \frac{1}{2} \omega_{\Pi} \quad (\Pi \text{ even})$$

$$P_{2i} = \frac{1}{2} (\omega_{2i} + \omega_{2i+1})$$

$$P_{2i+1} = \frac{1}{2} (\omega_{2i} - \omega_{2i+1})$$

The extension of the Fourier transform method to two dimensions is by two one-dimensional Fourier transforms.

3(iii) The use of cosine transforms requires that, at the boundaries, the derivatives of pressure are zero. The full problem has non-zero derivatives. To adapt the full problem into a homogeneous problem we use the linearity of the Poisson equation to pose two sub-problems and sum their solutions to find the full problem solution (Roache (1976) p 132). The two dimensional approach is the sum of one dimensional problems so we shall consider only one horizontal part of equation [1], (the vertical boundary conditions are imposed differently as is described in 3(iv)), ie

$$\frac{\partial^2 P}{\partial x^2} = S$$

$$\frac{\partial P}{\partial x} \Big|_{x=0} = g(0) \quad \frac{\partial P}{\partial x} \Big|_{x=Lx} = g(Lx) \quad [9]$$

Consider the sub problems

$$\frac{\partial^2 \phi_1}{\partial x^2} = S_1, \quad \frac{\partial \phi_1}{\partial x} = 0 \quad x=0, Lx \quad [10]$$

$$\frac{\partial^2 \phi_2}{\partial x^2} = S_2, \quad \frac{\partial \phi_2}{\partial x} = g(x) \quad x=0, Lx \quad [11]$$

then, since the system is linear,

$$\frac{\partial^2}{\partial x^2} (\phi_1 + \phi_2) = S_1 + S_2, \quad \frac{\partial}{\partial x} (\phi_1 + \phi_2) = g(x) \quad x=0, Lx$$

if we choose $\phi_2(i) = 0 \quad i=1, 2, \dots, \Pi$

and $\phi_2(0) = -g(0)\Delta x, \quad \phi_2(\Pi+1) = g(Lx)\Delta x$

then $\frac{\partial \phi_2}{\partial x} = g(x) \quad x=0, Lx$

and ϕ_2 satisfies equation [11] if

$$S_2(1) = -g(0) \frac{1}{\Delta x}$$

$$S_2(\Pi) = g(Lx) \frac{1}{\Delta x}$$

So, if we form $S_1 = S - S_2$ for $i = 1, II$ we can solve the homogeneous problem (equation [10]) and find P from

$$p_i = \phi_1(i) + \phi_2(i) \quad i = 0, 1, 2, \dots, II, II+1$$

3(iv) Returning to the full problem (equation [2]) and assuming that the horizontal boundaries have been reduced to the homogeneous form and the horizontal Fourier analysis has been performed we have

$$\nabla_H^2 \hat{P} + \frac{1}{DZ} \left\{ \frac{1}{DZN_{k+1}} (\hat{P}_{k+1} - \hat{P}_k) - \frac{1}{DZN} (\hat{P} - \hat{P}_{k-1}) \right\} + \frac{1}{2DZ} \left\{ \int \hat{P}_{k+1} - \int_{k-1} \hat{P}_{k-1} \right\} \quad [12]$$

$$= \hat{S}(\bar{i}, \bar{j})$$

where $\hat{P} = \hat{P}_{\bar{i}\bar{j}} \quad \bar{i} = 1, 2, \dots, II, \bar{j} = 1, 2, \dots, SS$

and $\nabla_H^2 \hat{P} = \left\{ \frac{\partial^2}{\partial \bar{x}^2} \left(\cos \frac{\pi}{II} (\bar{i}-1) - 1 \right) + \frac{\partial^2}{\partial \bar{y}^2} \left(\cos \frac{\pi}{SS} (\bar{j}-1) - 1 \right) \right\} \hat{P}(\bar{i}, \bar{j})$

The vertical boundary conditions become

$$\frac{\partial \hat{P}}{\partial \bar{z}} + \int \hat{P} = \hat{g}(\bar{z}) \quad \bar{z} = 0, H$$

ie $\frac{\hat{P}_2 - \hat{P}_1}{DZN_2} + \int \frac{1}{2} (\hat{P}_2 - \hat{P}_1) = \hat{g}_1$

and
$$\frac{\hat{p}_{kk} - \hat{p}_{kk-1}}{DZ N_{kk}} + \int_{kk-1}^k \frac{1}{2} (\hat{p}_{kk} - \hat{p}_{kk-1}) = \hat{g}_{kk-1}$$

or
$$\hat{p}_{kk} = \hat{h}(\bar{i}\bar{j})$$

We can write equation [12] as

$$\alpha_k \hat{p}_{k+1} + \beta_k(\bar{i}\bar{j}) \hat{p}_k + \gamma_k \hat{p}_{k-1} = \hat{s}_k \quad k=2, \dots, KK-1 \quad [13]$$

where

$$\alpha_k = \frac{1}{DZ} \left\{ \frac{1}{DZ N_{k+1}} + \frac{1}{2} \right\} \quad [14]$$

$$\beta_k(\bar{i}\bar{j}) = -\frac{1}{DZ} \left\{ \frac{1}{DZ N_{k+1}} + \frac{1}{DZ N} \right\} + \frac{\nabla_H^2 \hat{p}}{\hat{p}} \quad [15]$$

$$\gamma_k = \frac{1}{DZ} \left\{ \frac{1}{DZ N} - \frac{1}{2} \right\} \quad [16]$$

The solution to equation [13] can be written as (eg Potter (1973), p 88)

$$\hat{p}_k = \hat{p}_{k-1} \chi_{k-1} + y_{k-1} \quad [17]$$

where

$$x_{k-1} = \frac{\gamma_k}{(\alpha_k x_k + \beta_k)}$$

$$y_{k-1} = \frac{\hat{s}_k - \alpha_k y_k}{(\alpha_k x_k + \beta_k)}$$

To solve first scan down from $k = KK-1$ to $k = 2$, calculating x_k and y_k , starting with

$$x_{KK-1} = - \frac{(\frac{f_{KK-1}}{2} - \frac{1}{DZ N_{KK}})}{(\frac{f_{KK-1}}{2} + \frac{1}{DZ N_{KK}})}$$

$$y_{KK-1} = \frac{\hat{g}_{KK-1}}{(\frac{f_{KK-1}}{2} + \frac{1}{DZ N_{KK}})}$$

or with $x_{KK-1} = 0$, $y_{KK-1} = \hat{h}$

then scan upwards, obtaining \hat{p} from equation [17], starting with

$$\hat{p}_2 = \frac{\hat{g}_1 - [\frac{1}{DZ N_2} + \frac{f_1}{2}] y_1}{[\frac{f_1}{2} - \frac{1}{DZ N_2}] + [\frac{1}{DZ N_2} + \frac{f_1}{2}] x_1} \quad [18]$$

If the upper pressure is fixed there is no indeterminacy in the solution; or if $\frac{\partial f}{\partial \beta} \neq 0$ the solution is fully specified. However, if $\frac{\partial f}{\partial \beta} = 0$ equations [14] to [16] imply that $x_k(1,1) = 1$ ($k = 1, KK-1$) and thus from equation [18] $\hat{p}_2(1,1)$ is undefined, hence Neumann boundary conditions

require that $\hat{p}_2(1,1)$ be specified, though this specification has only numerical not dynamical significance. This recursive algorithm is vectorizable only in the horizontal direction (II*JJ points).

4. SUBROUTINE 'PRESNEU'

The subroutine assumes that the homogeneous problem (equation [10]) is to be solved and that the true P will be found elsewhere.

The FFT routines written by Temperton (1983) (now in Met 0 12 pool P12LIB) are used for the periodic transforms.

In order to maximise the vector length at each step (so that eg JJ vectors of length $KK \cdot II$ are transformed rather than KK times JJ transforms of length II) the data is reorganised at various stages using Q8VGATHR and Q8VSCATR. Initially the data is assumed to be stored as KK slices of length NIJ , in each of which the required $II \cdot JJ$ vector is embedded ie the subroutine begins with the P storage set up as

$$p(ijk) = p((k-1) \cdot NIS + (j-1) \cdot II + i) \quad [19]$$

but the y transform vector length is largest when P is stored as

$$p(ikj) = p((j-1) \cdot II \cdot KK + (k-1) \cdot II + i) \quad [20]$$

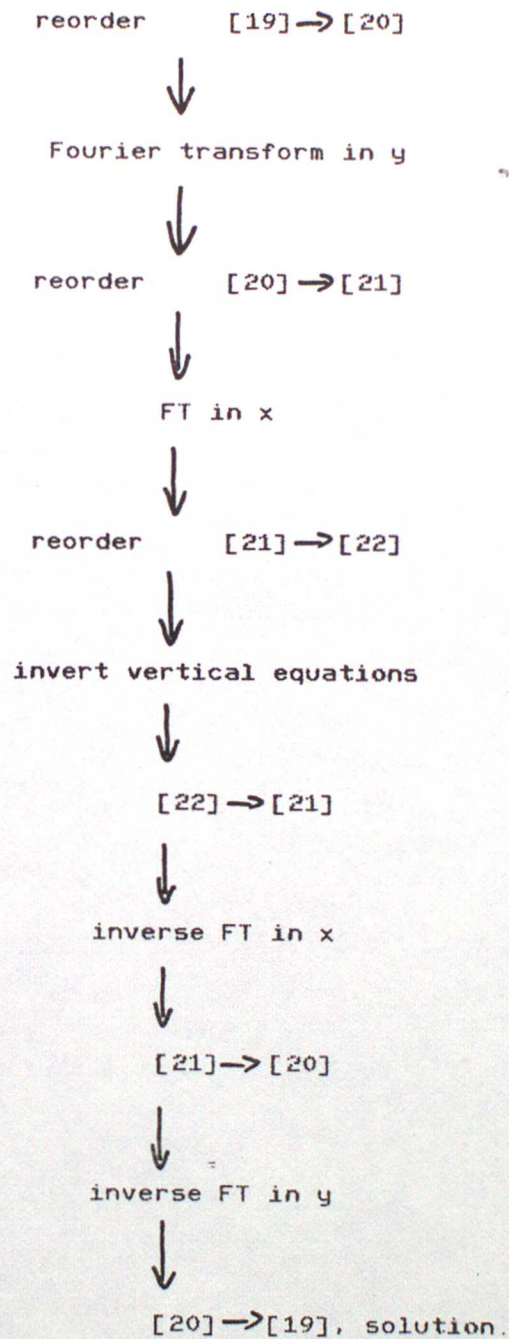
whilst the x Fourier transform vector length is maximised for

$$p(jki) = p((i-1) \cdot JJ \cdot KK + (k-1) \cdot JJ + j) \quad [21]$$

and the maximum contiguous vector for the vertical inversion is given when P is stored as,

$$p(i,k) = p((k-1)*II + (i-1)*JJ + j)_{[22]}$$

The structure of the subroutine is



A count of significant operations, ie those directly relevant to the solution and not the gather/scatter etc, using the values quoted by Temperton (1979) gives approximately

$$II * JJ * KK \{ 5 \log_2 II + 5 \log_2 JJ + 27 \}$$

operations per solution. For a 20 x 20 x 20 array the subroutines work at 80 MFLOPS (total time is 0.007 sec). This is approximately the same rate as the FFT subroutines (Temperton (1982)) and shows that the manipulations and tridiagonal solution do not degrade the solver speed.

The subroutine has been tested by using random data (acted on by the left hand side of equation [23]) as the source function. In all cases the original data was restored to 1 part in 10^9 (the error arising from the FFT subroutines).

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