

$$B = \begin{bmatrix} (1-\alpha)^2 & & & & & \\ & (1-\alpha)^2 & & & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & & \ddots & \\ & & & & & (1-\alpha)^2 \end{bmatrix}, \text{ and } \mathbf{f}_j = \begin{bmatrix} \alpha u_0(jl) \\ 0 \\ \vdots \\ 0 \\ \alpha u_1(jl) \end{bmatrix}.$$

In a similar way, we can treat the more accurate Crank–Nicholson finite difference method in which the term $\partial^2 u / \partial x^2$ in equation (2.1) is replaced by the average of the central difference operators on the lines $(j+1)l$ and jl .

It can be shown by a similar analysis to that given earlier that with the transformation,

$$r = 2\alpha / (1 - \alpha)^2 \quad (2.7)$$

or

$$\alpha = [(1 + 1/r) - \{(1 + 1/r)^2 - 1\}^{1/2}] \quad (2.8)$$

the finite difference equation for the Crank–Nicholson method becomes

$$-\alpha u_{i-1,j+1} + (1 + \alpha^2)u_{i,j+1} - \alpha u_{i+1,j+1} = \alpha u_{i-1,j} + (1 - 4\alpha + \alpha^2)u_{i,j} + \alpha u_{i+1,j}, \quad (2.9)$$

which when applied to the points $i = 1, 2, \dots, N - 1$ on each grid line gives a linear system of equations similar to (2.6) but with

$$B = \begin{bmatrix} \delta & \alpha & & & & \\ \alpha & \delta & \alpha & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \alpha \\ & & & & \alpha & \delta \end{bmatrix} \text{ and } \mathbf{f}_j = \begin{bmatrix} \alpha u_0(jl) + \alpha u_0((j+1)l) \\ 0 \\ \vdots \\ 0 \\ \alpha u_1(jl) + \alpha u_1((j+1)l) \end{bmatrix}$$

where $\delta = 1 - 4\alpha + \alpha^2$.

From the stability considerations of the two implicit methods discussed in this section, we know them to be stable and free from rounding error growth for all values of $r > 0$. This condition can be verified to be satisfied for all α in the range $0 < \alpha < 1$ for both equations (2.6) and (2.9).

The solution at each time step is usually obtained by solving the implicit equations (2.6) and (2.9) by a variant of Gaussian elimination (Varga, 1963). For large time integrations, this can involve a considerable amount of computation. However, in very many cases, the implicit equation (2.6) yields a matrix A which is often symmetric with constant coefficients, and the need for a special purpose algorithm can be justified particularly if the equations contain time varying constants $k(t)$ or if frequent changes in the time step Δt (and hence r) are envisaged which would require recomputation of the tridiagonal matrix algorithm. A further application is when implicit methods are used in a Stefan problem and the range of integration varies at each time step.

3. Applications to boundary value problems

In the numerical solution of quasi-linear parabolic and elliptic partial differential equations with constant or time varying coefficients involving two space dimensions and specified boundary conditions by the alternating direction implicit methods, there occurs a similar computational problem in which the ideas developed in Section 2 can be exploited.

For diffusion problems involving two space dimension, we consider a square region R with sides of length unity and mesh coordinates specified by (ih, jh) for $0 \leq i, j \leq N$ where $h = \Delta x = \Delta y = 1/N$, the mesh increment. The initial conditions are specified in the plane region R with boundary S . The differential equations and the boundary conditions are defined on the sets R' and S' of all points (x, y, t) such that $t \geq 0$ and $(x, y) \in R$ and such that $t \geq 0$ and $(x, y) \in S$

respectively. Thus, we consider the equation

$$\frac{\partial u}{\partial t} = k \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \quad (x, y, t) \in R' \quad (3.1)$$

with boundary and initial conditions

$$u(x, y, t) = g(x, y, t), \quad (x, y, t) \in S, \quad (3.2)$$

and

$$u(x, y, 0) = f(x, y), \quad (x, y) \in R. \quad (3.3)$$

A significant advance in the solution of such problems was made by Peaceman and Rachford (1955), who devised the method of alternating directions for solving the finite difference equations arising from (3.1). In this method, we use two forms of equation alternately in successive time steps; in the first the finite difference equations are implicit in the x -direction and explicit in the y -direction, and in the second the directions are interchanged.

Again, we use the relation

$$kl/h^2 = \alpha / (1 - \alpha)^2, \quad (3.4)$$

to simplify the implicit finite difference equations derived from (3.1) in the x - and y - directions to obtain,

$$-\alpha u_{i-1,j,2n+1} + (1 + \alpha^2)u_{i,j,2n+1} - \alpha u_{i+1,j,2n+1} = \alpha u_{i,j-1,2n} + (1 - 4\alpha + \alpha^2)u_{i,j,2n} + \alpha u_{i,j+1,2n}, \quad (3.5)$$

and

$$-\alpha u_{i,j-1,2n+2} + (1 + \alpha^2)u_{i,j,2n+2} - \alpha u_{i,j+1,2n+2} = \alpha u_{i-1,j,2n+1} + (1 - 4\alpha + \alpha^2)u_{i,j,2n+1} + \alpha u_{i+1,j,2n+1} \quad (3.6)$$

for all points $1 \leq i, j \leq N - 1$ and subject to the boundary conditions (3.2).

The equations (3.5) and (3.6) when grouped together yield the following pair of compound matrix systems,

$$E\mathbf{u}_{2n+1} = F\mathbf{u}_{2n} + \mathbf{g}_1 \quad (3.7)$$

and

$$E\tilde{\mathbf{u}}_{2n+2} = F\tilde{\mathbf{u}}_{2n+1} + \mathbf{g}_2$$

where E and F are compound matrices of order $(N - 1) \times (N - 1)$ and defined as

$$E = \begin{bmatrix} A & & & & \\ & A & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & A \end{bmatrix}_{N-1} \quad F = \begin{bmatrix} \delta I & \alpha I & & & \\ \alpha I & \delta I & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \alpha I \end{bmatrix}_{N-1}$$

with A , δ and \mathbf{f} as previously defined in Section 2 and \mathbf{u} , $\tilde{\mathbf{u}}$ are row-wise and column-wise compound vectors yielding the solution along rows and columns of the given domain R and \mathbf{g}_1 and \mathbf{g}_2 are vectors derived from the appropriate boundary conditions and ordered row-wise and column-wise accordingly.

Thus, we have shown that the alternating direction implicit methods can with a little analysis be expressed in a computational form whereby the tridiagonal systems which need to be solved along each row and column of the network can have a predetermined factorised form, thus eliminating the most tedious and time consuming part of the method.

Consider further then, for example, the second order elliptic partial differential equation

$$-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + 2\sigma u = f(x, y) \quad 0 < x, y < 1 \quad \sigma = \sigma(t) \quad (3.8)$$

in the unit square R with the Dirichlet boundary conditions,

$$u(x, y) = b(x, y), \quad (x, y) \in \partial R, \quad (3.9)$$

where b is specified on ∂R , the boundary of R . Writing (3.8) as

$$\left[-\frac{\partial^2 u}{\partial x^2} + \sigma u \right] + \left[-\frac{\partial^2 u}{\partial y^2} + \sigma u \right] = f, \quad (3.10)$$

where each term in brackets represents a differential operator

$$x_n = [g_n + \beta g_{n-1} + \dots + \beta^{n-1} g_1 - \beta^{n-1} (\beta \gamma) g_1 - \dots - \beta (\beta \gamma)^{n-1} g_{n-1} - (\beta \gamma)^n g_n] / [1 - (\beta \gamma)^{n+1}], \quad (4.8)$$

and

$$y_{n+1} = -\beta x_n.$$

Then, a back substitution process yields the components of the auxiliary solution,

$$y_i = g_i + \gamma y_{i+1} \text{ for } i = n, n-1, \dots, 2, 1, \quad (4.9)$$

whilst the components of the solution vector x are given by

$$x_1 = y_1$$

and a forward substitution of the form

$$x_i = y_i + \beta x_{i-1} \text{ for } i = 2, 3, \dots, n-1. \quad (4.10)$$

Since by definition $\beta, \gamma \leq |1|$, it follows immediately that the numerical processes defined by (4.8) to (4.10) are stable against the accumulation of rounding errors (Evans, 1972).

For the special case when $b = 2a = 2c$, and $\beta, \gamma = -1$ then equation (4.8) is indeterminate, and an alternative expression can be obtained. Thus, we have

$$x_n = [ng_n - (n-1)g_{n-1} + (n-2)g_{n-2} \dots + (-1)^{n-1} g_1] / (n+1) \quad (4.11)$$

together with

$$y_{n+1} = x_n, y_i = g_i - y_{i+1}, \text{ for } i = n, n-1, \dots, 2, 1, \quad (4.12)$$

and finally

$$x_1 = y_1, x_i = y_i - x_{i-1}, \text{ for } i = 2, 3, \dots, n-1. \quad (4.13)$$

5. ALGOL program

procedure tridiagsolv(n, a, b, c, d);

value n ;

integer n ;

real a, b, c ;

array d ;

comment Procedure solves the set of linear equations $Ax = d$ where the coefficient matrix is tridiagonal with constant sub-diagonal, diagonal and super-diagonal entries a, b, c respectively. During computation all the input vectors are over-written and the solution vector replaces d , the vector of constants. A work space of $(n+9)$ variables is used and the number of operations is of the order of

multiplications	4n
divisions	2n
additions	4n;

begin

integer i ;

array $y[1:n+1]$;

real $\beta, \beta n, \gamma, \delta, \text{sum1}, \text{sum2}, \text{res}, \text{eps}$;

$\delta := 0.5 \times (b + \text{sqrt}(b^2 - 4 \times a \times c))$;

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$\text{eps} := 0.000005$

$\beta := -a/\delta; \gamma := -c/\delta;$

for $i := 1$ **step** 1 **until** n **do**

$d[i] := d[i]/\delta;$

if $\text{abs}(\beta + 1.0) < \text{eps}$ **and** $\text{abs}(\gamma + 1.0) < \text{eps}$ **and** $\text{abs}(b^2 - 4 \times a \times c) < \text{eps}$ **then goto special**;

$\text{sum1} := 0;$

for $i := 1$ **step** 1 **until** n **do**

$\text{sum1} := d[i] + \text{sum1} \times \beta;$

$\beta n := \beta^n;$

$\text{sum2} := 0;$

for $i := n$ **step** -1 **until** 1 **do**

$\text{sum2} := d[i] + \text{sum2} \times \gamma;$

$\text{sum1} := \text{sum1} - \text{sum2} \times \beta n \times \gamma;$

$\beta n := (\beta \times \gamma)^{\uparrow (n+1)};$

$\text{res} := \text{sum1}/(1 - \beta n);$

$y[n+1] := -\beta \times \text{res};$

for $i := n$ **step** -1 **until** 1 **do**

$y[i] := d[i] + \gamma \times y[i+1];$

$d[1] := y[1];$

for $i := 2$ **step** 1 **until** $n-1$ **do**

$d[i] := y[i] + \beta \times d[i-1];$

$d[n] := \text{res};$

goto exit;

special : $\text{sum1} := d[1];$

for $i := 2$ **step** 1 **until** n **do**

$\text{sum1} := \text{sum1} - (-1)^{\uparrow i} \times i \times d[i];$

$\text{sum2} := (-1)^{\uparrow n} \times \text{sum1}/(n+1);$

$y[n+1] := -\text{sum2};$

for $i := n$ **step** -1 **until** 1 **do**

$y[i] := d[i] - y[i+1];$

$d[1] := y[1];$

for $i := 2$ **step** 1 **until** $n-1$ **do**

$d[i] := y[i] - d[i-1];$

$d[n] := y(n+1);$

exit : **end of tridiagsolv**;

6. Conclusions

Fast algorithmic solutions to the implicit difference equations of both initial and boundary value problems have been demonstrated to be feasible for equations with time varying constants or if frequent changes in the time step of integration is necessary. Further work is underway to increase the applicability of these ideas to problems involving more general boundary conditions. The manner in which they can be implemented has been briefly discussed previously by Evans (1966).

7. Acknowledgement

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