A Note on a Generalisation of a Method of Douglas

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1. Abstract and Introduction. In this note, the high-order correct method of Douglas [1] for the diffusion equation in one space variable is extended to $q \leqq 3$ space variables. The resulting difference equations are then solved using the A. D. I. technique of Douglas and Gunn [3]. When $q = 2$, this method is equivalent to that of Mitchell and Fairweather [5] while $q = 3$ provides a method which is similar to Samarskiĭ's method [6] and of higher accuracy than that of Douglas [2].

When the proposed methods are used to solve the diffusion equation with time-independent boundary conditions, they have the advantage that no boundary modification (see [4]) is required to maintain accuracy. ■

2. Derivation of Difference Equations. Consider the initial-boundary value problem

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \sum_{i=1}^{q} \frac{\partial^2 u}{\partial x_i^{\,2}}, \qquad (\mathbf{x}, t) \in R \times (0, T), \\
u(\mathbf{x}, 0) &= g(x), \qquad (\mathbf{x}, t) \in R \times \{0\}, \\
u(\mathbf{x}, t) &= f(\mathbf{x}, t), \qquad (\mathbf{x}, t) \in \partial R \times [0, T],
\end{aligned}
\tag{2.1}
$$

where $\mathbf{x} = (x_1, \cdots, x_q) \in [0, 1]^q \equiv I_q$, R is the interior of I_q and ∂R its boundary. A set of grid points with space increments $\Delta x_i = 1/h$, $(i = 1, \cdots, q)$ where $Nh = 1$ and time increment $\Delta t = T/M$ where N and M are integers is imposed on the region $\overline{R} \times [0, T]$, where $\overline{R} = R + \partial R$. Denote by w_n an approximation to $u(\mathbf{x}, t) = u_n$ at the grid point $(m_1 h, m_2 h, \cdots, m_q h, n\Delta t)$ where $m_i = 0, 1, \cdots, N$, $(i = 1, \cdots, q)$ and $n = 0, 1, \cdots, M$.

To derive the high order methods, we observe that

$$\frac{u_{n+1} - u_n}{\Delta t} = \left(\frac{\partial u}{\partial t}\right)_{n+1/2} + O((\Delta t)^2)$$

and

$$\left(\sum_{i=1}^{q} \frac{\partial^2 u}{\partial x_i^{\,2}}\right)_{n+1/2} = \frac{1}{2} \sum_{i=1}^{q} \Delta_{x_i}^2 (u_{n+1} + u_n) - \frac{h^2}{12} \sum_{i=1}^{q} \left(\frac{\partial^4 u}{\partial x_i^{\,4}}\right)_{n+1/2} + O(h^4 + (\Delta t)^2),$$

where $\Delta_{x_i}^2 = (1/h^2)\, \delta_{x_i}^2$, $\delta_{x_i}^2$ being the usual central difference operator.

Now

$$\sum_{i=1}^{q} \frac{\partial^4 u}{\partial x_i^{\,4}} = \left(\sum_{i=1}^{q} \frac{\partial^2}{\partial x_i^{\,2}}\right)^2 u - 2 \sum_{i=1;\, j>i}^{q-1} \frac{\partial^4 u}{\partial x_i^{\,2} \partial x_j^{\,2}}.$$

Thus

Received May 27, 1968.

$$\left(\sum_{i=1}^{q} \frac{\partial^4 u}{\partial x_i^{\,4}}\right)_{n+1/2} = \frac{1}{\Delta t} \sum_{i=1}^{q} \Delta_{x_i}^2 (u_{n+1} - u_n) - 2 \sum_{i=1;\, j>i}^{q-1} \Delta_{x_i}^2 \Delta_{x_j}^2 u_n + O(h^2 + (\Delta t)^2 + h^4/\Delta t)\,.$$

Hence if we set $r = \Delta t/h^2$, the scheme

$$\frac{w_{n+1} - w_n}{\Delta t} = \frac{1}{2} \sum_{i=1}^{q} \Delta_{x_i}^2 (w_{n+1} + w_n) - \frac{1}{12r} \sum_{i=1}^{q} \Delta_{x_i}^2 (w_{n+1} - w_n) + \frac{\Delta t}{6r} \sum_{i=1;\, j>i}^{q-1} \Delta_{x_i}^2 \Delta_{x_j}^2 w_n \tag{2.2}$$

is locally fourth-order correct in space and second-order correct in time.

By an analysis similar to that presented in [2] it can be shown that if $q \leqq 3$ the solution of the difference equation (2.2) converges in the mesh L_2 norm on R, the global discretisation error being fourth-order correct in space and second-order correct in time.

3. A. D. I. Technique. The use of (2.2) in practice would require the solution of a large system of linear equations at each time step. This problem may be simplified by the use of the Douglas-Gunn A. D. I. technique [3]. Equation (2.2) may be rewritten in the form

$$\left[1 - \frac{\Delta t}{2}\left(1 - \frac{1}{6r}\right) \sum_{i=1}^{q} \Delta_{x_i}^2\right] w_{n+1} - \left[1 + \frac{\Delta t}{2}\left(1 + \frac{1}{6r}\right) \sum_{i=1}^{q} \Delta_{x_i}^2 + \frac{1}{6r} (\Delta t)^2 \sum_{i=1;\, j>i}^{q-1} \Delta_{x_i}^2 \Delta_{x_j}^2\right] w_n = 0 \tag{3.1}$$

which can be solved by constructing a sequence $\beta_{n+1}^{(1)}, \cdots, \beta_{n+1}^{(q-1)}, \beta_{n+1}^{(q)} \equiv w_{n+1}$ of intermediate solutions in the following way:

$$\begin{gathered}\left[1 - \frac{\Delta t}{2}\left(1 - \frac{1}{6r}\right)\Delta_{x_1}^2\right]\beta_{n+1}^{(1)} \\ = \left[1 + \frac{\Delta t}{2}\left(1 + \frac{1}{6r}\right)\Delta_{x_1}^2 + \Delta t \sum_{i=2}^{q} \Delta_{x_i}^2 + \frac{(\Delta t)^2}{6r} \sum_{i=1;\, j>i}^{q-1} \Delta_{x_i}^2 \Delta_{x_j}^2\right] w_n \\ \left[1 - \frac{\Delta t}{2}\left(1 - \frac{1}{6r}\right)\Delta_{x_i}^2\right]\beta_{n+1}^{(i)} = \beta_{n+1}^{(i-1)} - \frac{\Delta t}{2}\left(1 - \frac{1}{6r}\right)\Delta_{x_i}^2 w_n\,, \\ i = 2, \cdots, q\,.\end{gathered} \tag{3.2}$$

Thus the intermediate solutions are obtained by solving only tridiagonal systems of equations.

It is interesting to note that if $q = 2$ and the intermediate solution $\beta_{n+1}^{(1)}$ is eliminated from (3.2) we obtain the formula derived in [5]. In a similar way, the formula presented by Samarskiĭ [6] is obtained from (3.2) when $q = 3$.

4. Stability and Accuracy of A. D. I. Method. The stability of (3.2) is proved by modifying Theorem 2.2 of [3]. This modification is necessary since the operators

$$A_i \equiv \left\{-\frac{\Delta t}{2}\left(1 - \frac{1}{6r}\right)\Delta_{x_i}^2\right\} \tag{4.1}$$

are not positive semidefinite for all values of r.

THEOREM. *Let* (3.1) *be written in the form*

$$(I + A)w_{n+1} + Bw_n = 0$$

where $A = \sum_{i=1}^{q} A_i$, A_i *given by* (4.1). *Since the difference operators* $A_1, \cdots, A_q, A$ *and* B *satisfy*

1. $I/q + A_i$ *is positive definite*, $i = 1, \cdots, q$,
2. B *is Hermitian*,
3. $A_1, \cdots, A_q, B$ *commute*,

the stability of (3.1) *implies the stability of* (3.2).

The proof follows the same lines as that of Douglas and Gunn if we make use of

LEMMA. *If* $I/q + A_i$ *is positive definite*, $i = 1, \cdots, q$, *then* $\sum_{2 \leq |\sigma| \leq q} A_\sigma$ *is positive semidefinite where* $\sigma = (i_1, i_2, \cdots, i_m)$, $i_1 < i_2 < \cdots < i_m$, $|\sigma| = m$ *and* $A_\sigma = A_{i_1} A_{i_2} \cdots A_{i_m}$.

That (3.2) is globally fourth-order correct in space and second-order correct in time is an immediate consequence of Theorem 2.3 of [3].

5. Intermediate Boundary Values. If the boundary conditions are time dependent the boundary conditions for the intermediate solutions $\beta_{n+1}^{(i)}$ $(i = 1, \cdots, q - 1)$ appearing in (3.2) must be chosen in a particular way in order that the global error of (3.2) remain $O(h^4 + (\Delta t)^2)$ otherwise a loss of accuracy will occur. For example, if $q = 2$ and the boundary values at the intermediate step are chosen to be those at the time level $(n + 1)\ \Delta t$, it can be shown that the global error is then $O((\Delta t)^2/h^{3/2} + h^4 + (\Delta t)^2)$ and if the boundary values at time level $(n + 1/2)\ \Delta t$ are chosen an even worse error results. To maintain the $O(h^4 + (\Delta t)^2)$ accuracy the boundary values at the intermediate step should be determined from the second of formulae (3.2) in the manner prescribed in [4]. If $q = 3$, accuracy can be maintained by carrying out a similar procedure.

It can also be shown using the techniques developed in [4] that no boundary modification is required at the intermediate levels when the boundary conditions are independent of time. In particular, formulae (3.2) with $q = 2$ can be used as an iterative method for solving Laplace's equation in two space variables without any cumbersome boundary modification like that required by the method proposed in [4]. The new procedure will provide more accurate approximations than the Peaceman-Rachford method [3] with little additional computational effort.

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