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 $q \leq 3$ 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 Samarskii's method [6] and of higher accuracy than that of Douglas [2].

When the proposed methods are used to solve the diffusion equation with timeindependent 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

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

where $\mathbf{x} = (x_1, \dots, x_q) \in [0, 1]^q \equiv I_q$, R is the interior of I_q and ∂R its boundary. A set of grid points with space increments $\Delta x_i = 1/h$, $(i = 1, \dots, q)$ where Nh = 1and 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 $(m_1h, m_2h, \dots, m_qh, n\Delta t)$ where $m_i = 0, 1, \dots, N$, $(i = 1, \dots, q)$ and $n = 0, 1, \dots, M$.

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

(2.1)

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

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

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

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

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

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 $q \leq 3$ 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

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

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:

$$\begin{bmatrix} 1 - \frac{\Delta t}{2} \left(1 - \frac{1}{6r} \right) \Delta_{x_1}^2 \end{bmatrix} \beta_{n+1}^{(1)} = \begin{bmatrix} 1 + \frac{\Delta t}{2} \left(1 + \frac{1}{6r} \right) \Delta_{x_1}^2 + \Delta t \sum_{i=2}^q \Delta_{x_i}^2 + \frac{(\Delta t)^2}{6r} \sum_{i=1; j>i}^{q-1} \Delta_{x_i}^2 \Delta_{x_j}^2 \end{bmatrix} w_n$$

$$\begin{bmatrix} 1 - \frac{\Delta t}{2} \left(1 - \frac{1}{6r} \right) \Delta_{x_i}^2 \end{bmatrix} \beta_{n+1}^{(i)} = \beta_{n+1}^{(i-1)} - \frac{\Delta t}{2} \left(1 - \frac{1}{6r} \right) \Delta_{x_i}^2 w_n ,$$

$$i = 2, \cdots, q ,$$

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 $\beta_{n+1}^{(\prime)}$ is eliminated from (3.2) we obtain the formula derived in [5]. In a similar way, the formula presented by Samarskii [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

(4.1)
$$A_{i} \equiv \left\{ -\frac{\Delta t}{2} \left(1 - \frac{1}{6r} \right) \Delta_{x_{i}}^{2} \right\}$$

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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, \dots, A_q, A_q and B satisfy

1. $I/q + A_i$ is positive definite, $i = 1, \dots, q$,

2. B is Hermitian,

3. A_1, \dots, 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, $i = 1, \dots, q$, then $\sum_{2 \le |\sigma| \le q} A_{\sigma}$ 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 $\beta_{n+1}^{(i)}$ $(i = 1, \dots, q-1)$ 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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