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 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

\[
\frac{\partial u}{\partial t} = \sum_{i=1}^{q} \frac{\partial^2 u}{\partial x_i^2}, \quad (x, t) \in R \times (0, T),
\]

\[
u(x, 0) = g(x), \quad (x, t) \in R \times \{0\},
\]

\[
u(x, t) = f(x, t), \quad (x, t) \in \partial R \times [0, T],
\]

where \( x = (x_1, \cdots, x_q) \in [0, 1]^q = I_q \), \( R \) is the interior of \( I_q \) and \( \partial R \) 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 \( R \times [0, T] \), where \( R = R + \partial R \). Denote by \( u_n \) an approximation to \( u(x, t) \) at the grid point \((m_1h, m_2h, \cdots, m_qh, n\Delta t)\) 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

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

where \( \Delta^2 x_i = (1/h^2) \delta^2_{x_i} \), \( \delta^2_{x_i} \) being the usual central difference operator.

Now

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

Thus

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\[
\left( \sum_{i=1}^{q} \frac{\partial^4 u}{\partial x_i^4} \right)_{n+1/2} = \frac{1}{\Delta t} \sum_{i=1}^{q} \Delta x_i^2 (u_{n+1} - u_n) - 2 \sum_{i=1, j>i}^{q-1} \Delta x_i^2 \Delta x_j^2 u_n + O(h^3 + (\Delta t)^3 + h^4/\Delta t). 
\]

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

\[
\frac{w_{n+1} - w_n}{\Delta t} = \frac{1}{2} \sum_{i=1}^{q} \Delta x_i^2 (w_{n+1} + w_n) - \frac{1}{12r} \sum_{i=1}^{q} \Delta x_i^2 (w_{n+1} - w_n)
\]

\[+ \frac{\Delta t}{6r} \sum_{i=1, j>i}^{q-1} \Delta x_i^2 \Delta x_j^2 w_n.
\]

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

\[
\left[ 1 - \frac{\Delta t}{2} \left( 1 - \frac{1}{6r} \right) \sum_{i=1}^{q} \Delta x_i^2 \right] w_{n+1} - \left[ 1 + \frac{\Delta t}{2} \left( 1 + \frac{1}{6r} \right) \sum_{i=1}^{q} \Delta x_i^2 \right] w_n = 0
\]

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

\[
\left[ 1 - \frac{\Delta t}{2} \left( 1 - \frac{1}{6r} \right) \Delta x_i^2 \right] \beta_{n+1}^{(1)} = \left[ 1 + \frac{\Delta t}{2} \left( 1 + \frac{1}{6r} \right) \Delta x_i^2 + \Delta t \sum_{i=2}^{q} \Delta x_i^2 + \frac{(\Delta t)^2}{6r} \sum_{i=1, j>i}^{q-1} \Delta x_i^2 \Delta x_j^2 \right] w_n
\]

\[+ \frac{\Delta t}{6r} \sum_{i=1, j>i}^{q-1} \Delta x_i^2 \Delta x_j^2 w_n.
\]

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 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

\[
A_i = \left\{ - \frac{\Delta t}{2} \left( 1 - \frac{1}{6r} \right) \Delta x_i^2 \right\}
\]
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 \( A = \sum_{i=1}^{q} A_i \), given by (4.1). Since the difference operators \( A_1, \ldots, A_q, A \) and \( B \) satisfy

1. \( I/q + A_i \) is positive definite, \( i = 1, \ldots, q, \)
2. \( B \) is Hermitian,
3. \( A_1, \ldots, A_q, B \) 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, \( i = 1, \ldots, q, \) then \( \sum_{2 \leq |\sigma| \leq q} A_\sigma \) is positive semidefinite where \( \sigma = (i_1, i_2, \ldots, i_m), \ i_1 < i_2 < \cdots < i_m, \ |\sigma| = m \) 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 \( \beta_{i+1,n}^{(j)} (i = 1, \ldots, q - 1) \) 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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