

A NEW EXPLICIT METHOD FOR THE DIFFUSION-CONVECTION EQUATION

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Abstract—We consider here the finite difference approximation to the diffusion-convection equation, from which new explicit formulae are obtained which are asymmetric. These explicit schemes can then be used to develop a new class of methods called Group Explicit as introduced in [2].

Theoretical aspects of the stability, consistency, convergence and truncation errors of this new class of methods is briefly discussed and numerical evidence presented to confirm our recommendations.

1 INTRODUCTION

Recently numerical methods involving both *explicit* and *implicit* schemes for the solution of the diffusion-convection equation, i.e.

$$\frac{\partial u}{\partial t} = \varepsilon \frac{\partial^2 u}{\partial x^2} - k \frac{\partial u}{\partial x}, \quad (1.1)$$

have been studied extensively. It is necessary for this equation to be treated separately from the ordinary diffusion equation because of the presence of spatial derivatives of first order.

Briefly, the implicit methods, i.e. Crank–Nicolson, etc. normally offer unconditionally stable schemes but require the solution of systems of equations at each time step. Meanwhile the explicit schemes usually suffer from a restrictive stability condition.

However, it can be shown that by using different combinations and types of approximation for the terms $\partial^2 u / \partial x^2$ and $\partial u / \partial x$ in (1.1), a class of stable semi-explicit schemes which is of similar structure to the semi-explicit schemes introduced in [3–6].

The simplicity of explicit methods of solution prompts us to seek such a method with increased stability characteristics and with the capability that the solution can be obtained at many points concurrently on the “next generation” array/parallel computers. The introduction of this new class of explicit method called the Group Explicit method will enable the explicit methods to compete with implicit methods on level terms again.

2 ASYMMETRIC EXPLICIT METHODS

We now consider equation (1.1) in the domain $(0, 1) \times (0, \infty)$ with the initial condition,

$$u(x, 0) = f(x), \quad 0 \leq x \leq 1, \quad (2.1a)$$

and boundary conditions,

$$\begin{aligned} u(0, t) &= g_0(t), \quad t > 0, \\ u(1, t) &= g_1(t), \quad t > 0 \end{aligned} \quad (2.1b)$$

As usual, the open-rectangular domain is covered by a rectangular grid, with spacing Δx , Δt in the x , t directions respectively. The values of Δx and Δt are assumed uniform throughout the region and the grid points (x, t) denoted by $x = x_i = i\Delta x$, $t = t_j = j\Delta t$, $i = 0, 1, 2, \dots, m$, $m = 1/\Delta x$ and $j = 0, 1, 2, \dots$.

Consider now the approximations to the partial derivatives in (1.1) at the point (i, j) of the grid, then

$$\frac{\partial u}{\partial t} \approx (u_{i,j+1} - u_{i,j})/\Delta t, \tag{2.2a}$$

and

$$\frac{\partial^2 u}{\partial x^2} \approx \left[\left(\frac{\partial u}{\partial x} \right)_{i+1/2,j} - \left(\frac{\partial u}{\partial x} \right)_{i-1/2,j} \right] / \Delta x, \tag{2.2b}$$

where we have used the usual forward difference approximation for $\partial u/\partial t$ and a central difference approximation for $\partial^2 u/\partial x^2 = \partial/\partial x(\partial u/\partial x)$

Now Saul'yev[3] replaces the term $(\partial u/\partial x)_{i-1/2,j}$ with $(\partial u/\partial x)_{i-1/2,j+1}$ and uses the obvious central difference approximations

$$\left(\frac{\partial u}{\partial x} \right)_{i+1/2,j} \approx (u_{i+1,j} - u_{i,j})/\Delta x,$$

and

$$\tag{2.3}$$

$$\left(\frac{\partial u}{\partial x} \right)_{i-1/2,j+1} \approx (u_{i,j+1} - u_{i-1,j+1})/\Delta x$$

When these approximations are substituted into the diffusion convection equation (1.1) the final result is the formula,

$$\begin{aligned} \left[1 + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \right] u_{i,j+1} - \left(\varepsilon r - \frac{kr\Delta x}{2} \right) u_{i+1,j+1} \\ = \left(\varepsilon r + \frac{kr\Delta x}{2} \right) u_{i-1,j} + \left[1 - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \right] u_{i,j}, \end{aligned} \tag{2.4}$$

with local truncation error (L T E) given by,

$$T_{2.4} = -\varepsilon \left(\frac{\Delta t}{\Delta x} \right) \frac{\partial^2 u}{\partial x \partial t} + \frac{\Delta t^2}{24} \frac{\partial^3 u}{\partial t^3} + \frac{k}{24} (\Delta t)^2 \frac{\partial^3 u}{\partial x \partial t^2} + \frac{k}{6} (\Delta x)^2 \frac{\partial^3 u}{\partial x^3} + \frac{k\Delta x \Delta t}{12} \frac{\partial^3 u}{\partial x \partial t^2}, \tag{2.5}$$

and requires for stability the condition,

$$0 < r \leq \frac{1}{k\Delta x}, \tag{2.6}$$

to be satisfied where $r = \Delta t/(\Delta x)^2$

This condition for stability is always rather favourable since with the values, $\varepsilon = k = 1.0$, $\Delta x = 0.1$ then $k\Delta x = 0.1$ which is always less restrictive than the condition for the classical explicit formula

In the same manner, another analogous asymmetric equation can be determined, which has the form,

$$\begin{aligned} -\left(\varepsilon r + \frac{kr\Delta x}{2} \right) u_{i-1,j+1} + \left[1 + \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \right] u_{i,j+1} \\ = \left[1 - \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \right] u_{i,j} + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) u_{i+1,j}, \end{aligned} \tag{2.7}$$

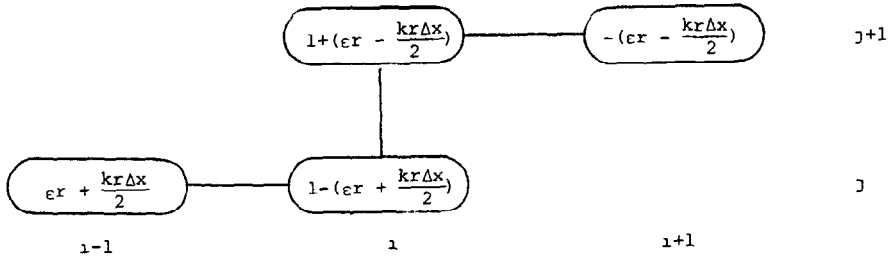


Fig 1

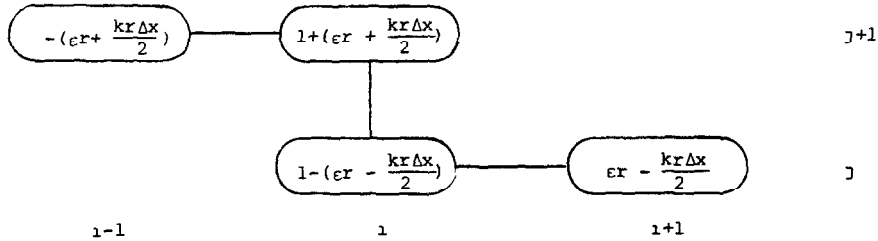


Fig 2

with the L T E given by,

$$T_{27} = \epsilon \left(\frac{\Delta t}{\Delta x} \right) \frac{\partial^2 u}{\partial x \partial t} + \frac{\Delta t^2}{24} \left[\frac{\partial^2 u}{\partial t^3} + k \frac{\partial^3 u}{\partial x \partial t^2} \right] + \frac{k}{6} (\Delta x)^2 \frac{\partial^3 u}{\partial x^3} - \frac{k \Delta x \Delta t}{12} \frac{\partial^3 u}{\partial x^2 \partial t} \quad (2.8)$$

For stability it requires the condition,

$$2\epsilon r(k\Delta x + 1) \geq 0, \quad (2.9)$$

to be satisfied, which is fulfilled by all values of $r > 0$ (Fig 2)

Due to the opposite signs of the truncation errors in (2.5) and (2.8), the following alternating direction explicit (ADE) algorithms which are similar to those suggested in [4] can be obtained by

- (1) Use of Equation (2.4) in a right-to-left direction (UNE)
- (2) Use of Equation (2.7) in a left-to-right direction (UPOS)
- (3) Use of Equation (2.4) at the j th time-level in a right-to-left direction and alternatively use of Equation (2.7) at the $(j + 1)$ th time-level in a left-to-right direction (ALDC)
- (4) Use of Equation (2.4) as in (1) and Equation (2.7) as in (2) at each time-level and then average the results (UAV)

Recently, an interesting new variation of the use of the asymmetric Equations (2.4) and (2.7) was investigated by the authors and reported in [2]. The central theme of the idea is not to restrict the use of Equations (2.4) and (2.7) solely along the x lines in the LR and RL directions but to apply them to groups of 2 points successively along each line in the manner as illustrated in Fig 3, where the symbol \circ denotes the use of Equation (2.4) and \square denotes the use of Equation (2.7)

The coupled use of Equations (2.4) and (2.7) at the points $(i, j + 1)$ and $(i + 1, j + 1)$ results in a (2×2) set of implicit finite difference equations which can be easily converted to explicit form as developed in the next section

3 GE FORMULATION AND ALGORITHMS

Consider now any two points $(i, j + 1)$ and $(i + 1, j + 1)$ and use Equation (2.4) at point $(i, j + 1)$ and use Equation (2.7) at point $(i + 1, j + 1)$ to give,

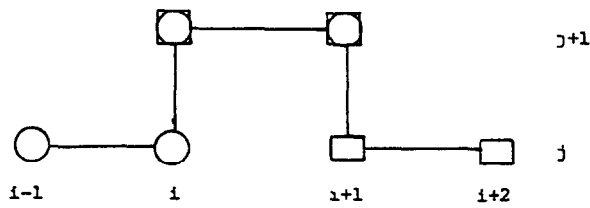


Fig 3

$$\begin{aligned} \left[1 + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \right] u_{i,j+1} - \left(\varepsilon r - \frac{kr\Delta x}{2} \right) u_{i+1,j+1} \\ = \left(\varepsilon r + \frac{kr\Delta x}{2} \right) u_{i-1,j} + \left[1 - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \right] u_{i,j}, \end{aligned} \quad (3.1)$$

and

$$\begin{aligned} - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) u_{i,j+1} + \left[1 + \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \right] u_{i+1,j+1} \\ = \left[1 - \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \right] u_{i+1,j} + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) u_{i+2,j}, \end{aligned} \quad (3.2)$$

respectively. Equations (3.1) and (3.2) will then form a small system of 2×2 linear equations, i.e.

$$\begin{aligned} \begin{bmatrix} 1 + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) & - \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \\ - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) & 1 + \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \end{bmatrix} \begin{bmatrix} u_{i,j+1} \\ u_{i+1,j+1} \end{bmatrix} \\ = \begin{bmatrix} 1 - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) & 0 \\ 0 & 1 - \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \end{bmatrix} \begin{bmatrix} u_{i,j} \\ u_{i+1,j} \end{bmatrix} + \begin{bmatrix} \left(\varepsilon r + \frac{kr\Delta x}{2} \right) u_{i-1,j} \\ \left(\varepsilon r - \frac{kr\Delta x}{2} \right) u_{i+2,j} \end{bmatrix} \end{aligned} \quad (3.3)$$

Since,

$$\begin{aligned} \begin{bmatrix} 1 + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) & - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \\ - \left(\varepsilon r + \frac{kr\Delta x}{2} \right) & 1 + \left(\varepsilon r + \frac{kr\Delta x}{2} \right) \end{bmatrix}^{-1} \\ = \frac{1}{1 + 2\varepsilon r} \begin{bmatrix} 1 + \left(\varepsilon r + \frac{kr\Delta x}{2} \right) & \varepsilon r - \frac{kr\Delta x}{2} \\ \varepsilon r + \frac{kr\Delta x}{2} & 1 + \left(\varepsilon r - \frac{kr\Delta x}{2} \right) \end{bmatrix} \end{aligned}$$

then (3.3) can be explicitly represented by,

$$\begin{aligned}
 & \begin{bmatrix} u_{i,j+1} \\ u_{i+1,j+1} \end{bmatrix} \\
 &= \frac{1}{(1 + 2\varepsilon r)} \left\{ \begin{bmatrix} 1 - \left(\varepsilon r + \frac{kr\Delta x}{2}\right)^2 & \left(\varepsilon r - \frac{kr\Delta x}{2}\right) \left[1 - \left(\varepsilon r - \frac{kr\Delta x}{2}\right) \right] \\ \left(\varepsilon r + \frac{kr\Delta x}{2}\right) \left[1 - \left(\varepsilon r + \frac{kr\Delta x}{2}\right) \right] & 1 - \left(\varepsilon r - \frac{kr\Delta x}{2}\right)^2 \end{bmatrix} \right. \\
 & \times \begin{bmatrix} u_{i,j} \\ u_{i+1,j} \end{bmatrix} + \left. \begin{bmatrix} \left(\varepsilon r + \frac{kr\Delta x}{2}\right) \left[1 + \left(\varepsilon r + \frac{kr\Delta x}{2}\right) \right] u_{i-1,j} + \left(\varepsilon r - \frac{kr\Delta x}{2}\right)^2 u_{i+2,j} \\ \left(\varepsilon r + \frac{kr\Delta x}{2}\right)^2 u_{i-1,j} + \left(\varepsilon r - \frac{kr\Delta x}{2}\right) \left[1 + \left(\varepsilon r - \frac{kr\Delta x}{2}\right) \right] u_{i+2,j} \end{bmatrix} \right\} \quad (3.4)
 \end{aligned}$$

In the case where there is any ungrouped point near either boundary, we use Equation (2.7), i.e.

$$\begin{aligned}
 u_{1,j+1} &= \frac{1}{\left[1 + \left(\varepsilon r + \frac{kr\Delta x}{2}\right) \right]} \\
 & \times \left\{ \left(\varepsilon r - \frac{kr\Delta x}{2}\right) u_{0,j+1} + \left[1 - \left(\varepsilon r - \frac{kr\Delta x}{2}\right) \right] u_{1,j} + \left(\varepsilon r - \frac{kr\Delta x}{2}\right) u_{2,j} \right\} \quad (3.5)
 \end{aligned}$$

for the left ungrouped point and Equation (2.4), i.e.

$$\begin{aligned}
 u_{m-1,j+1} &= \frac{1}{\left[1 + \left(\varepsilon r - \frac{kr\Delta x}{2}\right) \right]} \\
 & \times \left\{ \left(\varepsilon r - \frac{kr\Delta x}{2}\right) u_{m,j+1} + \left[1 - \left(\varepsilon r + \frac{kr\Delta x}{2}\right) \right] u_{m-1,j} + \left(\varepsilon r + \frac{kr\Delta x}{2}\right) u_{m-2,j} \right\}, \quad (3.6)
 \end{aligned}$$

for the right ungrouped point

To derive the algorithms which form the class of group explicit methods, we use the implicit form (3.3). Also we assume that the space interval x is divided into an even number of sub-intervals which implies that the value of $(m - 1)$ is odd. With the notations,

$$a_1 = \varepsilon - \frac{k\Delta x}{2},$$

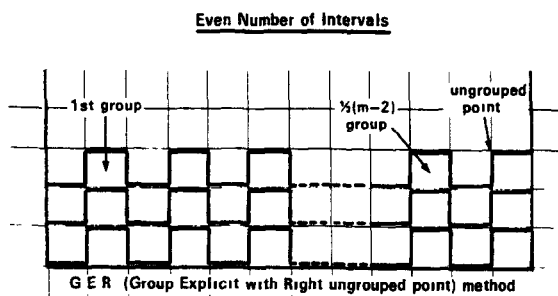


Fig 4

and

(3 7)

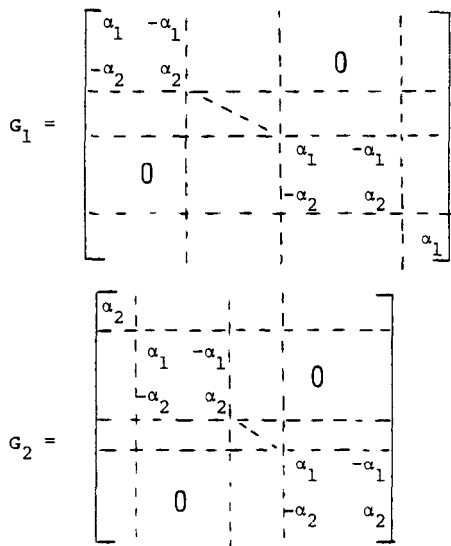
$$a_2 = \epsilon + \frac{k\Delta x}{2},$$

the following algorithms can be established

(1) *Group explicit with right-ungrouped point (GER)* Use Equation (3 3) for the first (m - 2) points and Equation (3 6) for the last unknown point (Fig 4) This will give the system,

$$(I + rG_1)\underline{u}_{j+1} = (I - rG_2)\underline{u}_j + \underline{b}_{1j}, \tag{3 8}$$

where,



$$\underline{b}_{1j}^T = [ra_2u_{0j}, 0, \dots, 0, ra_1u_{mj+1}]$$

and

$$\underline{u}_j^T = [u_{1j}, u_{2j}, \dots, u_{m-1j}]$$

(2) *Group explicit with left-ungrouped point (GEL)* Use Equation (3 5) for the first unknown point from the left of the boundary and Equation (3 3) for the remaining (m - 2)/ 2 pairs of points (Fig 5) This will result in the system,

$$(I + rG_2)\underline{u}_{j+1} = (I - rG_1)\underline{u}_j + \underline{b}_{2j}, \tag{3 11}$$

$$\text{with } \underline{b}_{2j}^T = [ra_2u_{0j+1}, 0, \dots, 0, ra_1u_{mj}]$$

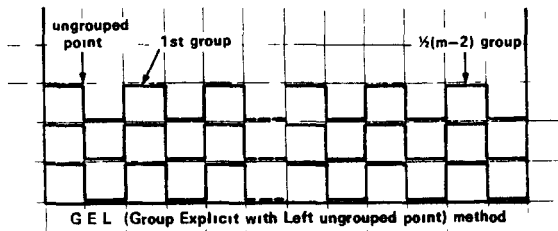


Fig 5

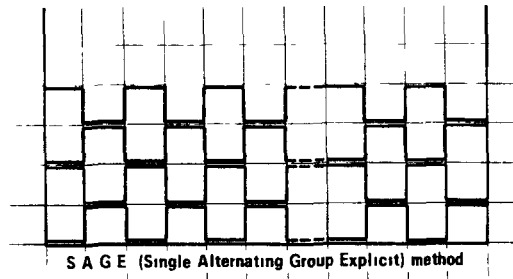


Fig 6

(3) *Alternating group explicit (S)AGE* Use Equation (3.8) at the $(j + 1)$ th time level and Equation (3.11) at the $(j + 2)$ th time level, (Fig. 6), i.e.

$$\begin{cases} (I + rG_1)u_{j+1} = (I - rG_2)u_j + b_{1j}, \\ (I + rG_2)u_{j+2} = (I - rG_1)u_{j+1} + b_{2j+1}, \end{cases} \quad (3.12)$$

(4) *Alternating group explicit (D)AGE* In this algorithm the group explicit formulae are incorporated alternately within the four time-levels with the direction reversed at the third time level (Fig. 7). This will give the equations,

$$\begin{aligned} (I + rG_1)u_{j+1} &= (I - rG_2)u_j + b_{1j}, \\ (I + rG_2)u_{j+2} &= (I - rG_1)u_{j+1} + b_{2j+1}, \\ (I + rG_2)u_{j+3} &= (I - rG_1)u_{j+2} + b_{2j+2}, \\ (I + rG_1)u_{j+4} &= (I - rG_2)u_{j+3} + b_{1j+3} \end{aligned} \quad (3.13)$$

These are only a few of the examples of the algorithms which can be established from the original formulae (3.4)–(3.6). There are a few more algorithms which the authors have omitted for brevity.

The estimate of the truncation errors of all the schemes mentioned is given in [1] and can be shown to be of order $O(\Delta t + (\Delta x)^2 + \Delta t/\Delta x)$. However, the (S)AGE and (D)AGE schemes are of the order $(\Delta t/\Delta x)^2$ with the consistency condition $(\Delta t/\Delta x) \rightarrow 0$ for $\Delta t \rightarrow 0, \Delta x \rightarrow 0$ applicable.

The stability analysis of this class of methods can be obtained by using the matrix method [1]. It was proved that the GER and GEL schemes are stable provided

$$r \leq \frac{1}{\max \left\{ \left| \varepsilon - \frac{k\Delta x}{2} \right|, \left| \varepsilon + \frac{k\Delta x}{2} \right| \right\}},$$

and for the (S)AGE and (D)AGE schemes they are unconditionally stable for all $r > 0$ provided $\Delta x \leq 2\varepsilon/k$.

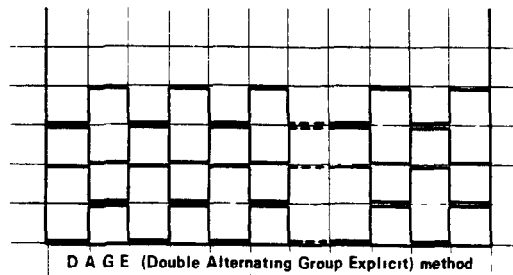


Fig 7

$k=1.0, \epsilon=1.0, \Delta t=0.005, \Delta x=0.1, r=0.5, t=0.5$

Method \ x	0.1	0.2	0.3	0.4
CNU	1.7×10^{-3}	3.2×10^{-3}	4.5×10^{-3}	5.4×10^{-3}
Eqn. 2.4 (UNE)	1.9×10^{-4}	3.5×10^{-4}	4.7×10^{-4}	5.2×10^{-4}
Eqn. 2.7 (UPOS)	3.3×10^{-4}	6.1×10^{-4}	8.1×10^{-4}	9.1×10^{-4}
ALDC Eqn. 2.4 & 2.7	1.1×10^{-4}	2.4×10^{-4}	3.6×10^{-4}	4.6×10^{-4}
AVERAGE Eqn. 2.4 & 2.7	0.7×10^{-4}	1.3×10^{-4}	1.7×10^{-4}	2.0×10^{-4}
(D) AGE	0.2×10^{-4}	0.6×10^{-4}	0.5×10^{-4}	0.8×10^{-4}
EXACT SOLUTION	0.06043	0.12730	0.20136	0.28345

0.5	0.6	0.7	0.8	0.9
6.1×10^{-3}	6.2×10^{-3}	5.8×10^{-3}	4.7×10^{-3}	2.8×10^{-3}
5.1×10^{-4}	4.4×10^{-4}	3.3×10^{-4}	2.0×10^{-4}	0.8×10^{-4}
9.1×10^{-4}	8.2×10^{-4}	6.5×10^{-4}	4.4×10^{-4}	2.2×10^{-4}
5.2×10^{-4}	5.3×10^{-4}	4.8×10^{-4}	3.8×10^{-4}	2.1×10^{-4}
2.0×10^{-4}	1.9×10^{-4}	1.6×10^{-4}	1.2×10^{-4}	0.7×10^{-4}
0.3×10^{-4}	0.8×10^{-4}	0.9×10^{-4}	0.6×10^{-4}	0.6×10^{-4}
0.37447	0.47539	0.58724	0.71114	0.84830

Table 1

$k=1.0, \epsilon=1.0, \Delta t=0.01, \Delta x=0.1, r=1.0, t=1.0$

Method \ x	0.1	0.2	0.3	0.4
CNU	1.5×10^{-3}	2.9×10^{-3}	4.1×10^{-3}	4.9×10^{-3}
Eqn. 3.1 (UNE)	2.4×10^{-5}	4.5×10^{-5}	6.3×10^{-5}	7.7×10^{-5}
Eqn. 3.4 (UPOS)	3.3×10^{-5}	6.2×10^{-5}	8.5×10^{-5}	10.3×10^{-5}
ALDC Eqn. 3.1 & 3.4	3.2×10^{-5}	6.2×10^{-5}	8.8×10^{-5}	10.8×10^{-5}
AVERAGE Eqn. 3.1 & 3.4	2.8×10^{-5}	5.3×10^{-5}	7.4×10^{-5}	9.0×10^{-5}
(D) AGE	2.7×10^{-5}	5.2×10^{-5}	7.2×10^{-5}	8.8×10^{-5}
EXACT SOLUTION	0.06120	0.12884	0.20360	0.28621

0.5	0.6	0.7	0.8	0.9
5.5×10^{-3}	5.7×10^{-3}	5.3×10^{-3}	4.3×10^{-5}	2.6×10^{-5}
8.6×10^{-5}	8.9×10^{-5}	8.4×10^{-5}	7.0×10^{-5}	4.3×10^{-5}
11.3×10^{-5}	11.4×10^{-5}	10.4×10^{-5}	8.4×10^{-5}	5.0×10^{-5}
12.1×10^{-5}	12.3×10^{-5}	11.5×10^{-5}	9.3×10^{-5}	5.5×10^{-5}
9.9×10^{-5}	10.1×10^{-5}	9.4×10^{-5}	7.7×10^{-5}	4.6×10^{-5}
9.8×10^{-5}	10.0×10^{-5}	9.4×10^{-5}	7.6×10^{-5}	4.6×10^{-5}
0.37752	0.47843	0.58996	0.71322	0.84945

Table 2

4 NUMERICAL EXAMPLE

In this example the equation (1.1) together with the initial condition $f(x) = 0$ and boundary conditions $g_0(t) = 0$ and $g_1(t) = 1$ is used as a model problem. This problem can be shown by the method of separation of variables to have the exact solution,

$$u(x, t) = \frac{e^{kx/\varepsilon} - 1}{e^{k/\varepsilon} - 1} + \sum_{n=1}^{\infty} \frac{(-1)^n n\pi}{(n\pi)^2 + \left(\frac{k}{2\varepsilon}\right)^2} e^{k(x-1)/2\varepsilon} \sin(n\pi x) e^{-[(n\pi)^2 + k^2/4\varepsilon]t} \quad (4.1)$$

The solution of some of the numerical schemes presented earlier have been compared with this exact solution in terms of their absolute errors. A comparison is also made with the Crank–Nicolson upwinding (CNU) scheme. The results are given in Tables 1 and 2 and graphically in Fig. 8.

From the tables and graph it can be seen that the results for this class of methods are much more accurate than the CNU method. For $r = 0.5$ the (D)AGE scheme appears to be better than any other scheme.

5 CONCLUSIONS

The explicit schemes (2.4) and (2.7) obtained from the generalised approximation are both very easy and economical to implement. As they are unconditionally stable in a practical sense and also accurate, therefore they are strongly recommended.

The GE schemes derived are also comparably accurate and strongly stable. For $r \leq 2.0$, the GE schemes ((D)AGE in particular) are to be recommended against the CNU schemes.

One point worth noting here is that this class of methods which is made up of approximations to $\partial u/\partial y$ by both forward and backward differences at different time levels is always superior than the CNU schemes where $\partial u/\partial x$ is always approximated by the backward difference.

The scheme discussed in this chapter can be easily extended and adapted for multi-dimensional problems.

Finally, we can establish that since the method is explicit and highly stable, it can be recommended as an alternative competitive method for solving the diffusion-convection equation.

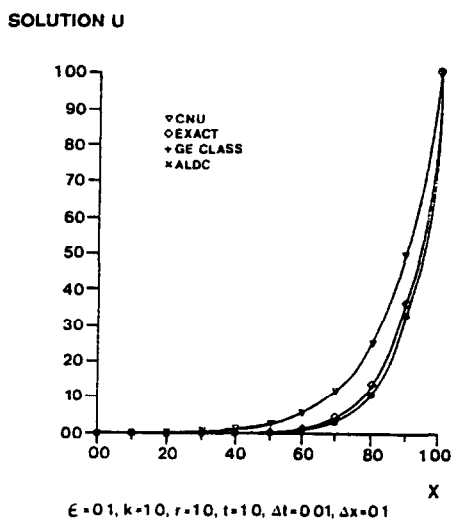


Fig. 8

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