# The Extrapolation of First Order Methods for Variable Coefficient Inhomogeneous Parabolic Partial Differential Equations 

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#### Abstract

The extrapolated Backward Euler method described by the authors in a previous paper is generalised to apply to both variable coeffient ard inhomogeneous partial differential equations of parabolic type. Methods of orders two, three and four are discussed.


## 1. Introduction

In previous papers (Lawson and Morris 1978, Gourlay and Morris 1980), the extrapolations of the Backward Euler method and the $\theta$ method have been considered for the numerical solution of homogeneous, constant coefficient parabolic partial differential equations.

In the paper of Lawson and Morris (1978), they derived second order accurate algorithms which exhibit $L_{0}$-stability. These algorithms appeared to produce promising results for problems in which discontinuities between initial and boundary conditions occurred. In comparison, it was found that the $A_{0}$-stable Crank-Nicolson method performed poorly on such problems. Consequently, in the paper of Gourlay and Morris (1980) they generalized the extrapolated scheme of Lawson and Morris (1978) to higher order: In particular, methods of order three and four were considered in some detail. It was found that amongst possible $L_{0}$ members of the family of methods, the schemes of orders three and four based on the Backward Euler method appeared to be most promising. Consequently, in the present paper we will use this basic algorithm to form the basis of the methods for parabolic differential equations in which the coefficients are time dependent and in which inhomogeneous, linear source terms are present.

## 2. Variable Coefficients

Consider the homogeneous self adjoint parabolic differential equation

$$
\begin{align*}
& \frac{\partial u}{\partial t}=\frac{\partial}{\partial x} a(x, t) \frac{\partial u}{\partial x} \quad(0<x<1) \times(t>0)  \tag{2.1}\\
& u(x, 0)=g(x) 0 \leq x \leq 1 ; u(0, t)=u(1, t)=0 \text { and } a(x, t)>0 \forall x, t .
\end{align*}
$$

In the usual manner, a discretization of the space variable $x$ is introduced. Let this be denoted by $h$ where $(N+1) h=1$ and the associated grid points are represented by $x_{i}=i h$.

At any grid point, let $\frac{\partial}{\partial x}$ be replaced by the central difference operator $\frac{\delta_{x}}{h}$ thereby introducing an error of $\boldsymbol{O}\left(h^{2}\right)$.

Hence, we may define $w$ to be defined by

$$
\begin{equation*}
\frac{d w}{d t}=\frac{1}{h^{2}} \delta_{x} a(x, t) \delta_{x} w \tag{2.2}
\end{equation*}
$$

where $x=x_{i}$. If eq. )2.2) is written for $\mathrm{i}=1,2, \ldots \mathrm{~N}$ we have

$$
\begin{equation*}
\frac{d \mathbf{w}}{d t}=A \mathbf{w} \tag{2.3}
\end{equation*}
$$

where $\mathbf{w}=\left(w_{1}, w_{2}, \ldots \ldots . . w_{N}\right)^{T}$ represents the vector of unknown values of the variable $w$ at the grid points $x_{i} i=1,2, \ldots N$ and the $(N \times N)$ matrix $\mathbf{A}$ is defined by

$$
\mathbf{A}=\frac{1}{h^{2}}\left[\begin{array}{cccccc}
-\bar{a}_{1} & a_{3 / 2} & & & & \\
a_{3 / 2} & -\bar{a}_{2} & a_{5 / 2} & & 0 & \\
& & \vdots & \vdots & \cdot & \\
& 0 & & \ddots & \ddots & a_{N-\frac{1}{2}} \\
& & & & a_{N-\frac{1}{2}} & -\bar{a}_{N}
\end{array}\right]
$$

where $\bar{a}_{i}=\left(a_{i+\frac{1}{2}}+a_{i-\frac{1}{2}}\right)$ and $a_{i} \equiv a\left(x_{i}, t\right)$. We note that the spatial dependency of the coefficient $a$ will have no bearing on the discussion in this paper and could equally well be omitted.

The elementary solution of eq (2.3) is given by

$$
\begin{equation*}
\mathbf{w}(t+2 \tau)=\exp \left[\int_{t}^{t+2 \tau} \mathbf{A}(\theta) d \theta\right] \mathbf{w}(t) \tag{2.4}
\end{equation*}
$$

In comparison, for the constant coefficient equation discussed by Gourlay and Morris (1980) we found

$$
\begin{equation*}
\mathbf{w}(t+2 \tau)=\exp [2 \tau \mathbf{A}] \mathbf{w}(t) \tag{2.5}
\end{equation*}
$$

(which is clearly reproduced by eq(2.4)). For eq(2.5) the second order algorithm proposed by Gourlay and Morris (1980), (with $\theta=0$ in the notation of that paper) is given by

$$
\begin{align*}
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(*)}=\mathbf{v}(t)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(1)}=\mathbf{v}^{(*)}}  \tag{2.6}\\
& {[\mathbf{I}-2 \tau \mathbf{A}] \mathbf{v}^{(2)}=\mathbf{v}(t)} \\
& \mathbf{v}(t+2 \tau)=2 \mathbf{v}^{(1)}-\mathbf{v}^{(2)}
\end{align*}
$$

and

For the variable coefficient problem represented by eq(2.4), in order to retain second order accuracy we clearly need to approximate to the argument $\int_{t}^{t+2 \tau} \mathbf{A}(\theta) d \theta$ to an order of accuracy consistent with this second order accuracy.

There are clearly many possibilities, the simplest of which appears to be the Mid-point rule

$$
\int_{t}^{t+2 \tau} \mathbf{A}(\theta) d \theta=2 \tau \mathbf{A}(t+\tau)+O\left(\tau^{3}\right) .
$$

This then, infers that the elements $a_{i}$ in $\mathbf{A}$ should be evaluated as $a(., t+\tau)$. The resulting second order algorithm is then given, simply, by eqs(2.6) with $\mathbf{A} \equiv$ $\mathbf{A}(\mathrm{t}+\tau)$ evaluated as indicated.

The third order algorithm proposed by Gourlay and Morris (1980) is given by

$$
\begin{align*}
& {[\mathbf{I}-\tau \mathbf{A}]^{3} \mathbf{v}^{(1)}=\mathbf{v}(t) } \\
& {[\mathbf{I}-2 \tau \mathbf{A}][\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(2)}=\mathbf{v}(t) }  \tag{2.7}\\
& \text { and } \quad[\mathbf{I}-3 \tau \mathbf{A}] \mathbf{v}^{(3)}=\mathbf{v}(t) \\
& \mathbf{v}(t+3 \tau)=\frac{9}{2} \mathbf{v}^{(1)}-\frac{9}{2} \mathbf{v}^{(2)}+\mathbf{v}^{(3) .}
\end{align*}
$$

Consequently, the integral in eq.(2.4) is required to third order accuracy. The natural choice for the quadrature is the Simpson $1 / 3$ rule so that

$$
\begin{equation*}
\int_{t}^{t+3 \tau} \mathbf{A}(\theta) d \theta=\frac{\tau}{2}\left[\mathbf{A}(t)+4 \mathbf{A}\left(t+3 \frac{\tau}{2}\right)+\mathbf{A}(3 \tau)\right]+O\left(\tau^{5}\right) \tag{2.8}
\end{equation*}
$$

This implies that the elements in the matrix A occurring in eq(2.7) are evaluated as

$$
\left(a(., t)+\frac{4}{3} a\left(., t+3 \frac{\tau}{2}\right)+a(., t+3 \tau)\right) / 6
$$

Finally, fourth order accuracy is obtained for the variable coefficient problem if $\mathbf{A}$ is defined in a similar manner to eq. (2.8), namely the elements $a_{i}$ in $\mathbf{A}$ should be evaluated as $(a(., t)+2 a(., t+2 \tau)+a(., t+4 \tau)) / 6$ and used in:

$$
\begin{align*}
& {[\mathbf{I}-\tau \mathbf{A}]^{4} \mathbf{v}^{(1)}=\mathbf{v}(t)} \\
& {[\mathbf{I}-3 \tau \mathbf{A}][\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(2)}=\mathbf{v}(t)} \\
& {[\mathbf{I}-2 \tau \mathbf{A}]^{2} \mathbf{v}^{(3)}=\mathbf{v}(t)}  \tag{2.9}\\
& {[\mathbf{I}-2 \tau \mathbf{A}][\mathbf{I}-\tau \mathbf{A}]^{2} \mathbf{v}^{(4)}=\mathbf{v}(t)} \\
& {[\mathbf{I}-4 \tau \mathbf{A}] \mathbf{v}^{(5)}=\mathbf{v}(t)}
\end{align*}
$$

and

$$
\mathbf{v}(t+4 \tau)=\alpha \mathbf{v}^{(1)}+\beta \mathbf{v}^{(2)}+\gamma \mathbf{v}^{(3)}+\delta \mathbf{v}^{(4)}+(1-\alpha-\beta-\gamma-\delta) \mathbf{v}^{(5)}
$$

There is considerable choice of the parameters here. However, Gourlay and Morris (1980) suggest $(\alpha, \beta, \gamma, \delta)=(8,40 / 9,0,-32 / 3)$ or $(0,16 / 9,-6,16 / 3)$.

The constant coefficient analysis for stability carried by Gourlay and Morris (1980) is unaffected by the variable coefficients present in the current paper so that the algorithms presented here all $L_{0}$-stable. However, we note the comments about variable coefficient problems solved using constant coefficient analysis discussed by Lambert (1979).

## 3. Inhomogeneous Problems

Consider the inhomogeneous parabolic differential equation.

$$
\begin{equation*}
\frac{\partial u}{\partial t}=k \frac{\partial^{2} u}{\partial x^{2}}+s(x, t) ;(0<x<1) \times(t>0) \tag{3.1}
\end{equation*}
$$

$u(x, 0)=g(x) ; u(0, t)=\mathbf{u}(1, t)=0$ and $k$ is a given constant. $s(x, t)$ is a given, possibly discontinuous, heat source.

The replacement of the second order derivative using the central differences produces the ordinary differential equation for the semi discrete approximation $\mathbf{w}$

$$
\begin{equation*}
\frac{d \mathbf{w}}{d t}=\mathbf{A w}+\mathbf{s}(t) \tag{3.2}
\end{equation*}
$$

where $\mathbf{s}=\left(s_{1}, s_{2}, \ldots \ldots, s_{N}\right)^{\tau}$ where $s_{i} \equiv s\left(x_{i}, t\right)$. The $N \times N$ matrix $\mathbf{A}$ is defined in section 2 with $a_{i} \equiv k$.

The solution of this ordinary differential equation is

$$
\begin{equation*}
\mathbf{w}(t+2 \tau)=\exp [2 \tau \mathbf{A}] \mathbf{w}(t)+\int_{t}^{t+2 \tau} \exp [(t+2 \tau-\theta) \mathbf{A}] \mathbf{s}(\theta) d \theta \tag{3.3}
\end{equation*}
$$

Consequently, to achieve orders of accuracy consistent with the homogeneous algorithms, the integral term in eq.(3.3) will have to be approximated to at least the order of the approximation to $\exp (\tau \mathbf{A})$. For second order, this is a simple task. Consider the extrapolated $\theta$-method with the introduction of the source term defined by

$$
\begin{align*}
& {[\mathbf{I}-\tau(1-\theta) \mathbf{A}] \mathbf{v}^{\left({ }^{*}\right)}=[\mathbf{I}+\tau \theta \mathbf{A}] \mathbf{v}(t)+\tau[(1-\theta) \mathbf{s}(t+\tau)+\theta \mathbf{s}(t)]} \\
& {[\mathbf{I}-\tau(1-\theta) \mathbf{A}] \mathbf{v}^{(1)}=[\mathbf{I}+\tau \theta \mathbf{A}] \mathbf{v}^{(*)}+\tau[(1-\theta) \mathbf{s}(t+2 \tau)+\theta \mathbf{s}(t+\tau)]}  \tag{3.4}\\
& {[\mathbf{I}-2 \tau(1-\theta) \mathbf{A}] \mathbf{v}^{(2)}=[\mathbf{I}+2 \tau \theta \mathbf{A}] \mathbf{v}(t)+2 \tau[(1-\theta) \mathbf{s}(t+2 \tau)+\theta \mathbf{s}(t)] .}
\end{align*}
$$

and

$$
\mathbf{v}(t+2 \tau)=\alpha \mathbf{v}^{(1)}+(1-\alpha) \mathbf{v}^{(2)}
$$

It is found that second order accuracy is obtained if

$$
\alpha=2 \forall \theta \text { or } \theta=\frac{1}{2} \forall \alpha
$$

To obtain third order accuracy, it is found that the natural extension of eq.(3.4) given by

$$
[\mathbf{I}-\tau(1-\theta) \mathbf{A}] \mathbf{v}^{(*)}=[\mathbf{I}+\tau \theta \mathbf{A}] \mathbf{v}(t)+\tau[(1-\theta) \mathbf{s}(t+\tau)+\theta \mathbf{s}(t)]
$$

$$
\begin{aligned}
& {[\mathbf{I}-\tau(1-\theta) \mathbf{A}] \mathbf{v}^{(* *)}=[\mathbf{I}+\tau \theta \mathbf{A}] \mathbf{v}^{(*)}+\tau[(1-\theta) \mathbf{s}(t+2 \tau)+\theta \mathbf{s}(t+\tau)]} \\
& {[\mathbf{I}-\tau(1-\theta) \mathbf{A}] \mathbf{v}^{(1)}=[\mathbf{I}+\tau \theta \mathbf{A}] \mathbf{v}^{(* *)}+\tau[(1-\theta) \mathbf{s}(t+3 \tau)+\theta \mathbf{s}(t+2 \tau)]} \\
& {[\mathbf{I}-2 \tau(1-\theta) \mathbf{A}] \mathbf{v}^{(2)}=[\mathbf{I}+\tau \theta \mathbf{A}] \mathbf{v}^{(*)}+2 \tau[(1-\theta) \mathbf{s}(t+3 \tau)+\theta \mathbf{s}(t+\tau)]} \\
& {[\mathbf{I}-3 \tau(1-\theta) \mathbf{A}] \mathbf{v}^{(3)}=[\mathbf{I}+3 \tau \theta \mathbf{A}] \mathbf{v}(t)+3 \tau[(1-\theta) \mathbf{s}(t+3 \tau)+\theta \mathbf{s}(t)]} \\
& \mathbf{v}(t+3 \tau)=\alpha \mathbf{v}^{(1)}+\beta \mathbf{v}^{(2)}+(1-\alpha-\beta) \mathbf{v}^{(3)}
\end{aligned}
$$

attains this order only for $\theta=\frac{1}{2}, 4 \alpha+3 \beta=\frac{9}{2}$. The $L_{0}$-stable member of this family occurs for $\alpha=\frac{3}{4}$ and hence, $\beta=\frac{1}{2}$. For any other value of $\theta$, in particular $\theta=0$, the method does not attain third order in its present form. To achieve third order the following possibilities exist.
(1) Take different weightings of the quadrature terms in eq.(3.4). For example using $\theta=0$;

$$
\begin{align*}
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(*)}=\mathbf{v}(t)+a \tau \mathbf{s}(t+\tau)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(*)}=\mathbf{v}^{(*)}+b \tau \mathbf{s}(t+2 \tau)} \\
& \left.[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(1)}=\mathbf{v}^{(* *}\right)+c \tau \mathbf{s}(t+3 \tau)  \tag{3.5}\\
& {[\mathbf{I}-2 \tau \mathbf{A}] \mathbf{v}^{(2)}=\mathbf{v}^{(*)}+d \tau \mathbf{s}(t+3 \tau)} \\
& {[\mathbf{I}-3 \tau \mathbf{A}] \mathbf{v}^{(3)}=\mathbf{v}(t)+e \tau \mathbf{s}(t+3 \tau)} \\
& \mathbf{v}(t+3 \tau)=\alpha \mathbf{v}^{(1)}+\beta \mathbf{v}^{(2)}+(1-\alpha-\beta) \mathbf{v}^{(3)}
\end{align*}
$$

where the parameters $a, b, c, d, e$ are to be chosen to give third order, we find the following equations must be satisfied in order that the expansion of $\mathbf{v}(t+3 \tau)$ given by eq. (3.5) agrees with the expansion of $\mathbf{w}(t+3 \tau)$

$$
\begin{array}{r}
a+c-d+\frac{2}{9} e=\frac{2}{3} \\
a+2 c-2 d+\frac{2}{3} e=1 \\
a-b+3 c-4 d+2 e=1
\end{array}
$$

Whereas this is an underdetermined system of equations, it is straight forward to verify that the system is inconsistent. Hence, this generalization is not feasible.
(2) Take the same weightings of the quadrature term in eq.(3.4) evaluating the data points at other points in time. Thus, with $\theta=0$ we propose

$$
\begin{align*}
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(*)}=\mathbf{v}(t)+\tau \mathbf{s}(t+a \tau)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(* *)}=\mathbf{v}^{(*)}+\tau \mathbf{s}(t+b \tau)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(1)}=\mathbf{v}^{\left({ }^{* *}\right)}+\tau \mathbf{s}(t+c \tau)}  \tag{3.5a}\\
& {[\mathbf{I}-2 \tau \mathbf{A}] \mathbf{v}^{(2)}=\mathbf{v}^{\left({ }^{( }\right)}+2 \tau \mathbf{s}(t+d \tau)} \\
& {[\mathbf{I}-3 \tau \mathbf{A}] \mathbf{v}^{(3)}=\mathbf{v}(t)+3 \tau \mathbf{s}(t+e \tau)}
\end{align*}
$$

and

$$
\mathbf{v}(t+3 \tau)=\frac{9}{2} \mathbf{v}^{(1)}-\frac{9}{2} \mathbf{v}^{(2)}+\mathbf{v}^{(3)}
$$

The parameters $a, \ldots, e$ now have to satisfy:

$$
\begin{gathered}
c+b-2 d+\frac{2}{3} e=1 \\
c+2 b-4 d+2 e=1 \\
c^{2}+b^{2}-2 d^{2}+\frac{2}{3} e^{2}=2
\end{gathered}
$$

which we note is independent of the parameter $a$. Since the source term is evaluated at $t+a \tau$ it is reasonable to choose a value of $a$ in the range [0,1]. For smooth problems, this choice of range produced no significant effect in the accuracy of the computed results. (However, see the comments in section 4). We would, however, recommend against choosing 'unreasonable' values of $a$ as it is clear that although the order of accuracy is independent of $a$ the error constant will depend on this parameter and values of $a$ not in $[0,1]$ should be avoided.

This system has an infinite number of solutions. Consequently, we recommend choosing values of the parameters which are convenient (rationals) and spread the integration points over the interval. Two sets which satisfy this criterion are:

$$
\begin{aligned}
& (i)(a), b=1, c=2, d=3 / 2, e=3 / 2 \\
& (i i)(a), b=3, c=2, d=5 / 2, e=3 / 2
\end{aligned}
$$

Hence, third order accurate variants of the extrapolated backward Euler method exist for the inhomogeneous problems. There remains to discuss the introduction of source terms into the order four methods discussed by Gourlay and Morris (1980). Using their algorithm for the homogeneous problem, we suggest the inhomogeneous algorithm given by:

## Define

$$
\begin{aligned}
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(*)}=\mathbf{v}(t)+\tau \mathbf{s}(t+a \tau)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{\left({ }^{* *}\right)}=\mathbf{v}^{\left.\mathbf{v}^{*}\right)}+\tau \mathbf{s}(t+b \tau)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{\left({ }^{* * *}\right)}=\mathbf{v}^{\left({ }^{* *}\right)}+\tau \mathbf{s}(t+c \tau)} \\
& {[\mathbf{I}-\tau \mathbf{A}] \mathbf{v}^{(1)}=\mathbf{v}^{\left({ }^{* * *}\right)}+\tau \mathbf{s}(t+d \tau)} \\
& {[\mathbf{I}-3 \tau \mathbf{A}] \mathbf{v}^{(2)}=\mathbf{v}^{(*)}+3 \tau \mathbf{s}(t+e \tau)} \\
& {[\mathbf{I}-2 \tau \mathbf{A}] \mathbf{v}^{(+)}=\mathbf{v}(t)+2 \tau \mathbf{s}(t+f \tau)} \\
& {[I-2 \tau \mathbf{A}] \mathbf{v}^{(3)}=\mathbf{v}^{(+)}+2 \tau \mathbf{s}(t+g \tau)} \\
& {[\mathbf{I}-2 \tau \mathbf{A}] \mathbf{v}^{(4)}=\mathbf{v}^{(* *)}+2 \tau \mathbf{s}(t+h \tau)} \\
& {[\mathbf{I}-4 \tau \mathbf{A}] \mathbf{v}^{(5)}=\mathbf{v}(t)+4 \tau \mathbf{s}(t+i \tau)}
\end{aligned}
$$

and then

$$
\begin{equation*}
\mathbf{v}(t+4 \tau)+\alpha \mathbf{v}^{(1)}+\beta \mathbf{v}^{(2)}+\gamma \mathbf{v}^{(3)}+\delta \mathbf{v}^{(4)}+(1-\alpha-\beta-\gamma-\delta) \mathbf{v}^{(5)} \tag{3.6}
\end{equation*}
$$

The conditions imposed in order that the homogeneous method is of order four and $L_{0}$ stable are those of Gourlay and Morris (1980)

$$
\begin{equation*}
8-6 \alpha-3 \beta-4 \gamma-5 \delta=0 \quad \text { and } \quad 2 \alpha+\delta=16 / 3 \tag{3.7}
\end{equation*}
$$

and

$$
16 / 3+\alpha-3 \beta=0
$$

The variable $\mathbf{v}$ in eq.(3.6) is to approximate to order four the variable $\mathbf{w}$ given by

$$
\begin{equation*}
\mathbf{w}(t+4 \tau)=\exp (4 \tau \mathbf{A}) \mathbf{w}(t)+\int_{t}^{t+4 \tau} \exp [(t+4 \tau-\theta) \mathbf{A}] \mathbf{s}(\theta) d \theta . \tag{3.8}
\end{equation*}
$$

With the condition indicated above in eq.(3.7) the term $\exp (4 \tau \mathbf{A}) \mathbf{w}(t)$ is approximated to order four. Consequently, it is required to choose the parameters ( $a, b$, $\ldots, i$ ) in eq.(3.6) in order that the terms in s agree with the expansion of the integral term in eq.(3.8), namely with

$$
\begin{align*}
& 4 \tau\left[\mathbf{I}+2 \tau \mathbf{A}+\frac{8}{3} \tau^{2} \mathbf{A}^{2}+\frac{8}{3} \tau^{3} \mathbf{A}^{3}\right] \mathbf{s}+\frac{8}{3} \tau^{3}\left[3 \mathbf{I}+4 \tau \mathbf{A}+4 \tau^{2} \mathbf{A}^{2}\right] \frac{\partial \mathbf{s}}{\partial t}+ \\
& \frac{32}{3} \tau^{3}[\mathbf{I}+\tau \mathbf{A}] \frac{\partial^{2} \mathbf{s}}{\partial t^{2}}+\frac{32}{3} \tau^{4} \frac{\partial^{3} \mathbf{s}}{\partial t^{3}} . \tag{3.9}
\end{align*}
$$

Owing to the number of parameters present in eq.(3.6), we use values of $\alpha, \beta, \gamma$ and $\delta$ given by the experiments of Gourlay and Morris (1980) for the homogeneous problem namely

$$
(\alpha, \beta, \gamma, \delta)=(8,40 / 9,0,-32 / 3) .
$$

Consequently, the expression of terms in eq.(3.6) will be independent of $g$ and $f$. So, in eq.(3.9), there are 10 expressions which must be reproduced by the expansion of eq.(3.6) which contains 6 parameters. However, the four terms in the expression

$$
\begin{equation*}
4 \tau\left[\mathbf{I}+2 \tau \mathbf{A}+\frac{8}{3} \tau^{2} \mathbf{A}^{2}+\frac{8}{3} \tau^{3} \mathbf{A}^{3}\right] \tag{3.10}
\end{equation*}
$$

should be produced independently of the parameters $a, b, \ldots, i$ provided the order four conditions (3.7) are satisfied. Carrying out the expansions of eq.(3.6) and gathering terms, we find that expression (3.10) is indeed given independently of $a, b, \ldots, i$. In addition, equating coefficients of the expansions of eq.(3.6) and the remaining terms in eq.(3.9), the following conditions must be satisfied in order that eq.(3.6) is fourth order accurate:

$$
\begin{array}{r}
\frac{2}{9} a-\frac{b}{3}+c+d+\frac{5}{3} e-\frac{8}{3} h-\frac{7}{18} i=1 \\
\frac{8}{9} a-b+2 c+d+5 e-\frac{16}{3} h-\frac{14}{9} i=\frac{4}{3} \\
\frac{23}{9} a-\frac{10}{3} b+3 c+d+15 e-\frac{32}{3} h-\frac{56}{9} i=\frac{4}{3} \\
\frac{2}{9} a^{2}-\frac{1}{3} b^{2}+c^{2}+d^{2}+\frac{5}{3} e^{2}-\frac{8}{3} h^{2}-\frac{7}{18} i^{2}=\frac{8}{3}  \tag{3.11}\\
\frac{8}{9} a^{2}-b^{2}+2 c^{2}+d^{2}+5 e^{2}-\frac{16}{3} h^{2}-\frac{14}{9} i^{2}=\frac{8}{3} \\
\frac{2}{9} a^{3}-\frac{b^{3}}{3}+c^{3}+d^{3}+\frac{5}{3} e^{3}-\frac{8}{3} h^{3}-\frac{7}{18} i^{3}=8
\end{array}
$$

a system of six nonlinear equations in seven unknowns. To solve this system we used a nonlinear system solver and specified $i$ as a parameter. We demand that the solution produce values of $a, b, \ldots, i$ between 0 and $4-$ any solution not satisfying this requirement is deemed unacceptable. The following is a table of values obtained - all of which give fourth order accuracy. Unfortunately, as can be seen, we were unable to obtain 'nice' values as was the case for the third order algorithm. In all cases listed in the table, the solutions were calculated in double precision arithmetic when the equations (3.11), on substituting the found values, were found to be exact to rounding error.

Table 3.1. (to six decimal places).

| a | b | c | d | e | h | i |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.408427 | 0.763474 | 1.309624 | 2.432547 | 1.347753 | 1.732872 | 1.666667 |
| 0.922536 | 3.165201 | 1.924524 | 2.857166 | 2.634664 | 2.454360 | 2.000000 |
| 0.885623 | 3.490869 | 2.111856 | 3.043468 | 2.879755 | 2.685641 | 2.125000 |
| 0.892726 | 3.918795 | 2.315610 | 3.299657 | 3.214382 | 2.983981 | 2.333333 |
| 0.898682 | 3.998700 | 2.347486 | 3.346771 | 3.276487 | 3.036850 | 2.375000 |
| 0.697906 | 1.173393 | 1.697287 | 2.738072 | 2.601413 | 2.444377 | 3.000000 |
| 0.390746 | 1.044248 | 2.049900 | 3.196421 | 3.489170 | 3.091799 | 4.000000 |

## 4. Numerical Experiments

In the current section, we will describe a small sample of the numerical experiments carried out using the novel algorithms described in the previous sections. The experiments have, essentially, been carried out to test the accuracy and $L_{0}$-stability.

For accuracy experiments, we considered it essential to separate the spatial discretization errors from those related to the time discretization. To test the algorithms of section 2 we chose to consider the following system of two linear ordinary differential equations:

$$
\begin{align*}
& \frac{d \mathbf{u}}{d t}=\mathbf{A u} \\
& \mathbf{u}(1.0)=(1.0,1.0) \text { with } \mathbf{A}=\left[\begin{array}{cc}
\chi / t & 0 \\
0 & \chi / t
\end{array}\right] \text { and } \mathbf{u}(t)=\left(t^{\chi}, t^{\chi}\right) \tag{4.1}
\end{align*}
$$

We computed the solution to $t=3.4$ for a large number of different parameter values; a sample set of the results is described here. The results we present are representative of the results obtained for the allowable parameter sets described in section 2 . We considered a sequence of values of $\chi$; we describe only those results for $\chi=-4$ similar behaviour being observed for other values of $\chi$. The various methods were run for a sequence of values of $\tau$ defined by $\tau=0.8 / 2^{i}$ for increasing $i$. The error at $\mathrm{t}=3.4$ and where applicable, its ratio to that obtained for the preceding value of $\tau$ is described in Tables 4.1-4.3. The ratios consistent with orders 2,3 and 4 in tables $4.1,4.2$ and 4.3 respectively would be 4,8 and 16 . This is seen to be the case in the third column of these tables. The numerical results are seen to confirm the accuracy of the schemes for the variable coefficients. In table 4.2, we also include the results obtained using a sequence of values of $\tau=$ $0.6 / 2^{i}$; this set of results is included to facilitate a comparison with diagonally implicit Runge Kutta methods described, for example, by Zlatev (1980) and Alexander (1977); the details of which are given below. We expand on the reason for this sequence of values of $\tau$ after introducing the 'competing' schemes. To our knowledge, the most competitive schemes described in the literature are the diagonally implicit Runge Kutta (DIRK) methods; see Alexander (1977), Zlatev (1980) as well as Norsett (1982) and Burrage et al. (1980). In Zlatev's MDIRK method (1980), a modified diagonally implicit Runge Kutta method was introduced which ensured the coefficient matrix which occurs at each time step is common to all stages; this ensures the resulting method is as efficient as possible. If we denote the ordinary differential equation being solved by

$$
\begin{equation*}
\frac{d \mathbf{y}}{d t}=\mathbf{A}(t) \mathbf{y}+\mathbf{s}(t) \tag{4.2}
\end{equation*}
$$

then Zlatev's MDIRK method can be defined as advancing the solution a single step of size $\tau$ from $t_{n}$ to $t_{n}+\tau$ by the formula

$$
\begin{align*}
& {\left[\mathrm{I}-\tau\left(1-\frac{\sqrt{ } 2}{2}\right) \mathbf{A}\left(t_{n}+\tau / 2\right)\right] \mathbf{y}_{n, 1}=\mathbf{A}\left(t_{n}+\tau / 2\right) \mathbf{y}_{n}+\mathbf{s}\left(t_{n}+\tau / 2\right)}  \tag{4.3}\\
& {\left[\mathbf{I}-\tau\left(1-\frac{\sqrt{ } 2}{2}\right) \mathbf{A}\left(t_{n}+\tau / 2\right)\right] \mathbf{y}_{n, 2}=\mathbf{A}\left(t_{n}+\tau / 2\right)\left[\mathbf{y}_{n}+\tau(\sqrt{ } 2-1) \mathbf{y}_{n, 1}\right]+\mathbf{s}\left(t_{n}+\tau / 2\right)} \\
& \mathbf{y}_{n+1}=\mathbf{y}_{n}+\frac{\tau}{2}\left[\mathbf{y}_{n, 1}+\mathbf{y}_{n, 2}\right]
\end{align*}
$$

where $\mathbf{y}_{n}$ is the approximation to $\mathbf{y}\left(t_{n}\right)$.
The coefficient matrix I $-\tau\left(1-\frac{\sqrt{2}}{2}\right) \mathbf{A}\left(t_{n}+\tau / 2\right)$ is common to both stages and so a single LU factorisation per time step is all that is needed. We note that in order to determine $\mathbf{y}_{n+1} 1 \mathrm{LU}$ decomposition, 2 forward/backward solves and 2 matrix/vector multiplications are required to advance the solution a single time step of size $\tau$. In this analysis of complexity, we have assumed the vector $\mathbf{A y}$ is calculated each time it is required. Clearly, this can be avoided if the first calculation of this vector also stores it. This increases the resulting storage requirements and we assume this is to be avoided. In the following comparisons, we have not compared the algorithms on the basis of storage requirements; the DIRK methods are much less efficient than the novel schemes because of the different matrices occurring in the algorithms; the novel methods merely need a modification of the diagonal entries. However, we base the comparison of arithmetic operations assuming each method is programmed using minimal computer storage. If this assumption is not valid, then the actual number of arithmetic operations will be slightly different; where appropriate we include in brackets the corresponding complexity. If we compare the second order method (2.6) with the above MDIRK scheme, we find 2 LU factorisations, 3 forward/backward solves and 0 matrix/vector multiplications are required to advance the solution over a step of size $2 \tau$. For partial differential equations, where $\mathbf{A}$ is banded, the matrix/vector multiplication is often of the same order of complexity as the LU factorisation and also the same order as the forward/ backward solves. So, in this context, we see the relative 'costs' are given in the first row of table 4.4 where (2.6) is used as defined and the comparable MDIRK is (4.3) with $2 \tau$, i.e. (2.6) is either twice as efficient as (4.3) or for the same complexity (4.3) should be written with $\tau$ replaced by $2 \tau$; we prefer the latter strategy as the basis of comparison. In table 4.1, we include the results obtained for eq(4.1) ( $\mathbf{s} \equiv \mathbf{0}$ ) by the MDIRK scheme (4.3). In comparing the accuracy betweem the two methods, because (4.3) is computed with $2 \tau$ where (2.6) computes with $\tau$ we compare the entries $i$ for (2.6) with entries $i-1$ for (4.3). Thus, we see, for example, for $i=8(2.6)$ the error is $0.143_{-5}$ and for $i=7$ (4.3) the error is $0.302_{-6}$; under the assumption that the computational complexity is the same we
see the novel scheme is less accurate than the MDIRK scheme for the homogeneous problem.

Table 4.1. Results for second order schemes.

| $\mathbf{i}$ | error | ratio | error | ratio |
| :---: | :---: | :---: | :---: | :---: |
| 3 | $0.824_{-3}$ |  | $0.794_{-4}$ |  |
| 4 | $0.266_{-3}$ | 3.09 | $0.196_{-4}$ | 4.06 |
| 5 | $0.779_{-4}$ | 3.42 | $0.485_{-5}$ | 4.03 |
| 6 | $0.213_{-4}$ | 3.66 | $0.121_{-5}$ | 4.01 |
| 7 | $0.559_{-5}$ | 3.81 | $0.302_{-6}$ | 4.00 |
| 8 | $0.143_{-5}$ | 3.90 | $0.753_{-7}$ | 4.00 |

Algorithm $2.6(\alpha=2, \theta=0)$ MDIRK (4.3)

$$
\tau=0.8 / 2^{i}
$$

Likewise a two stage third order (A-stable) DIRK scheme (Alexander 1977) can be proposed: define for eq.(4.2)

$$
\begin{align*}
& {\left[\mathrm{I}-\tau a_{1,1} \mathbf{A}\left(t_{n}+\tau_{1}\right)\right] \mathbf{y}_{n, 1}=\mathbf{y}_{n}+\tau a_{1,1} \mathbf{s}\left(t_{n}+\tau_{1}\right)} \\
& {\left[\mathbf{I}-\tau a_{2,2} \mathbf{A}\left(t_{n}+\tau_{2}\right)\right] \mathbf{y}_{n, 2}=\mathbf{y}_{n}+\tau a_{2,1}\left[\mathbf{A}\left(t_{n}+\tau_{1}\right) \mathbf{y}_{n, 1}+\mathbf{s}\left(t_{n}+\tau_{1}\right)\right]+\tau a_{2,2} \mathbf{s}\left(t_{n}+\tau_{2}\right)} \\
& \mathbf{y}_{n+1}=\mathbf{y}_{n}+\tau\left[b_{1}\left[\mathbf{A}\left(t_{n}+\tau_{1}\right) \mathbf{y}_{n, 1}+\mathbf{s}\left(t_{n}+\tau_{1}\right)\right]+b_{2}\left[\mathbf{A}\left(t_{n}+\tau_{2}\right) \mathbf{y}_{n, 2}+\mathbf{s}\left(t_{n}+\tau_{2}\right)\right]\right]  \tag{4.4}\\
& a_{1,1}=a_{2,2}=\frac{1}{2}+\frac{1}{2 \sqrt{ } 3}, a_{2,1}=\frac{-1}{\sqrt{3}} ; \tau_{1}=\frac{1}{2}+\frac{1}{2 \sqrt{ } 3} ; \tau_{2}=\frac{1}{2}-\frac{1}{2 \sqrt{ } 3}
\end{align*}
$$

and $b_{1}=b_{2}=1 / 2$.
The computational complexity of this method (4.4) is summarised in row 4 of table 4.4 and compares with the third order method which is the subject of the present paper, eq. (2.7) as indicated in row 3. Because (2.7) produces the solution at an increment of $3 \tau$ we run (4.4) with $\tau$ replaced by $3 \tau$ to make the computational costs equivalent. In this case, to continue to produce the solution at $t=3.4$ we ran (4.4) with a sequence of $\tau=0.6 / 2^{i}$. The results are summarised in table 4.2. Again to compare the results of the two methods, the error for (2.7) for $\tau=0.1$ should be compared with the error for (4.4) with $\tau=0.3$, namely row $i$ for (2.7) compares with the error in row $i-2$ for (4.4). Thus, for example, the error 0.548 _9 for (2.7) corresponding to $i=10$ compares with $0.669_{-9}$ for (4.4) in row $i=8$. As can be seen, for the same computational effort, the novel method appears to be competitive with the DIRK scheme.

Table 4.2. Results for third order methods.

| $\mathbf{i}$ | error | ratio | error | ratio |
| :---: | :---: | :---: | :---: | :---: |
| 3 | $0.295_{-3}$ |  | $0.177_{-4}$ |  |
| 4 | $0.660_{-4}$ | 4.47 | $0.246_{-5}$ | 7.22 |
| 5 | $0.118_{-4}$ | 5.58 | $0.325_{-6}$ | 7.56 |
| 6 | $0.182_{-5}$ | 6.51 | $0.419_{-7}$ | 7.77 |
| 7 | $0.254_{-6}$ | 7.16 | $0.531_{-8}$ | 7.88 |
| 8 | $0.336_{-7}$ | 7.55 | $0.669_{-9}$ | 7.94 |
| 9 | $0.432_{-8}$ | 7.77 |  |  |
| 10 | $0.548_{-9}$ | 7.88 |  |  |

Scheme (3.5a) $\alpha=-\beta=4.5 \theta=0$ DIRK (4.4)

$$
\tau=0.8 / 2^{i} \quad \tau=0.6 / 2^{i}
$$

Finally, we also compared the novel fourth order methods of this paper with a three stage fourth order $\mathbf{A}$-stable (DIRK) method described in Alexander (1977) namely;

$$
\begin{aligned}
& {\left[\mathbf{I}-\tau a_{1,1} \mathbf{A}\left(t_{n}+\tau_{1}\right)\right] \mathbf{y}_{n, 1}=\mathbf{y}_{n}+\tau a_{1,1} \mathbf{s}\left(t_{n}+\tau_{1}\right)} \\
& {\left[\mathbf{I}-\tau a_{2,2} \mathbf{A}\left(t_{n}+\tau_{2}\right)\right] \mathbf{y}_{n, 2}=\mathbf{y}_{n}+\tau a_{2,1}\left[\mathbf{A}\left(t_{n}+\tau_{1}\right) \mathbf{y}_{n, 1}+\mathbf{s}\left(t_{n}+\tau_{1}\right)\right]+\tau a_{2,2} \mathbf{s}\left(t_{n}+\tau_{2}\right)} \\
& {\left[\mathbf{I}-\tau a_{3,3} \mathbf{A}\left(t_{n}+\tau_{3}\right)\right] \mathbf{y}_{n, 3}=\mathbf{y}_{n}+\tau a_{3,1}\left[\mathbf{A}\left(t_{n}+\tau_{1}\right) \mathbf{y}_{n, 1}+\mathbf{s}\left(t_{n}+\tau_{1}\right)\right]} \\
& +\tau a_{3,2}\left[\mathbf{A}\left(t_{n}+\tau_{2}\right) \mathbf{y}_{n, 2}+\mathbf{s}\left(t_{n}+\tau_{2}\right)\right]+\tau a_{3,3} \mathbf{s}\left(t_{n}+\tau_{3}\right)
\end{aligned}
$$

$$
\begin{align*}
& \mathbf{y}_{n+1}=\mathbf{y}_{n}+\tau\left[b_{1}\left(\mathbf{A}\left(t_{n}+\tau_{1}\right) \mathbf{y}_{n, 1}+\mathbf{s}\left(t_{n}+\tau_{1}\right)\right)+b_{2}\left(\mathbf{A}\left(t_{n}+\tau_{2}\right) \mathbf{y}_{n, 2}+\right.\right.  \tag{4.5}\\
& \left.\left.\mathbf{s}\left(t_{n}+\tau_{2}\right)\right)+b_{3}\left(\mathbf{A}\left(t_{n}+\tau_{3}\right) \mathbf{y}_{n, 3}+\mathbf{s}\left(t_{n}+\tau_{3}\right)\right)\right]
\end{align*}
$$

where

$$
\begin{aligned}
& a_{1,1}=a_{2,2}=a_{3,3}=(1+\alpha) / 2 \\
& a_{2,1}=-\alpha / 2, a_{3,1}=1+\alpha, a_{3,2}=-(1+2 \alpha) \\
& \tau_{1}=(1+\alpha) / 2, \tau_{2}=1 / 2 \operatorname{and} \tau_{3}=(1-\alpha) / 2 . \\
& b_{1}=1 /\left(6 \alpha^{2}\right), b_{2}=1-1 /\left(3 \alpha^{2}\right), b_{3}=1 /\left(6 \alpha^{2}\right)
\end{aligned}
$$

and

$$
\alpha=\frac{2}{\sqrt{ } 3} \cos (\pi / 18)
$$

The errors obtained in solving (4.1) using (4.5) are summarised in table 4.3. Because (2.9) produces a solution at intervals of $4 \tau$, the comparable entries in table 4.3 are row $i$ for (2.9) and row ( $i-2$ ) for (4.5). Thus, for example, the error arising from (2.9) for $\tau=0.0125(i=6)$ compares with $\tau=0.05(i=4)$ for (4.5); so, again for comparable computational effort, the novel scheme appears to be most competitive.

Table 4.3. Results for fourth order schemes.

| $\mathbf{i}$ | error | ratio | error | ratio |
| ---: | :---: | :---: | :---: | :---: |
| 4 | $0.121_{-4}$ |  | $0.123_{-5}$ |  |
| 5 | $0.155_{-5}$ | 7.85 | $0.925_{-7}$ | 13.3 |
| 6 | $0.144_{-6}$ | 10.8 | $0.640_{-8}$ | 14.5 |
| 7 | $0.111_{-7}$ | 12.9 | $0.421_{-9}$ | 15.2 |
| 8 | $0.766_{-9}$ | 14.3 | $0.270_{-10}$ | 15.8 |
| 9 | $0.513_{-10}$ | 15.1 | $0.171_{-11}$ | 15.8 |
| 10 | $0.330_{-11}$ | 15.6 | $0.108_{-12}$ | 15.9 |

Method $3.6 \alpha=8, \beta=40 / 9, \gamma=0, \delta=-32 / 3$ DIRK 4.5

$$
\tau=0.8 / 2^{i}
$$

Table 4.4. Relative complexities of novel and DIRK schemes.

| Order | Method | D | F/B | Mv |
| :---: | :---: | :---: | :---: | :---: |
| Second | $(2.6)$ | 2 | 3 | 0 |
|  | $(4.3)$ | 1 | 2 | $3(2)$ |
| Third | $(2.7)$ | 3 | 5 | 0 |
|  | $(4.4)$ | 2 | 2 | $3(2)$ |
| Fourth | $(2.9)$ | 4 | 7 | 0 |
|  | $(4.5)$ | 3 | 3 | $6(3)$ |

Key: D:matrix decompositions; F/B; forward-backward solves; Mv: Matrix-vector multiplications.

For the inhomogeneous problem described in section 3, we chose to consider the following system of two ordinary differential equations:

$$
\begin{equation*}
\frac{d \mathbf{u}}{d t}=\mathbf{A u}+\mathbf{s} \tag{4.6}
\end{equation*}
$$

$\mathbf{u}(1.0)$ given where $\mathbf{A}=\left[\begin{array}{ll}2 & -1 \\ 3 & -2\end{array}\right] \mathbf{s}=\left(\chi t^{x^{-1}}-t^{x}, \chi t^{x-1}-t^{x}\right)^{T}$
and $\mathbf{u}(t)=\left(t^{\chi}, t^{\chi}\right)$.

In the results, we quote only the results for $\chi=-4$. Results for other values were similar. The various methods were run until $\mathrm{t}=3.4$ with time step $\tau=0.8 / 2^{j}$ for $\mathrm{j}=0,1, \ldots, 10$ and estimates of the exponent of $\tau$ made. Since $\tau$ was in each case being reduced by a factor of $1 / 2$ we would expect, for second order methods, that the error would be reduced at each stage by a factor close to 4 . This is clearly shown in sample table 4.5 for $\theta=0, \alpha=2$.

Similar results obtain for the other allowable choices of these parameters. The corresponding results for the third order method with $\theta=0.5$ are similar and not quoted. (It was noted that the choice $\alpha=9 / 8, \beta=0$ gave a fourth order error reduction ratio.) In the case of the third order method with $\theta=0$ and the first set of parameters third order behaviour as shown in table 4.6 was noted. Further, all the parameter sets identified in table 3.1 were found to give fourth order convergence when algorithm (3.6) was used. A sample set of results for the first set of parameters is given in table 4.7. We also carried out a comparison of the novel schemes with the DIRK methods (4.3), (4.4) and (4.5); the results are summarised in tables $4.5,4.6$ and 4.7 ; for table 4.6 the DIRK scheme (4.4) was run for the sequence of $\tau$ given by $\tau=0.6 / 2^{i}$ for the reasons explained earlier. For the computational complexity, the entries in the tables are compared as follows:

Table 4.5; method (3.4) error in row $i$ compared with method (4.3) error in row $i-1$.

Table 4.6; method (3.5a) error in row $i$ compared with method (4.4) error in row $i-2$.

Table 4.7; method (3.6) error in row $i$ compared with method (4.5) error in row $i-2$.

We see again that the novel schemes seem to be most competitive.

Table 4.5. Errors for second order algorithms.

| $\mathbf{i}$ | error | ratio | error | ratio |  |
| :--- | :--- | :--- | :--- | :--- | :---: |
| 3 | $0.142_{0}$ |  | $0.124_{0}$ |  |  |
| 4 | $0.358_{-1}$ | 3.98 | $0.312_{-1}$ | 3.96 |  |
| 5 | $0.863_{-2}$ | 4.15 | $0.782_{-2}$ | 3.99 |  |
| 6 | $0.210_{-2}$ | 4.11 | $0.196_{-2}$ | 4.00 |  |
| 7 | $0.516_{-3}$ | 4.07 | $0.489_{-3}$ | 4.00 |  |
| 8 | $0.128_{-3}$ | 4.04 | $0.122_{-3}$ | 4.00 |  |
| Method (3.4) DIRK (4.3) |  |  |  |  |  |
| $\tau=0.8 / 2^{i}$ |  |  |  |  |  |

Table 4.6. Errors for third order methods.

| $\mathbf{i}$ | error | ratio | error | ratio |
| ---: | :--- | :--- | :--- | :--- |
| 5 | $0.148_{-2}$ |  | $0.211_{-4}$ |  |
| 6 | $0.157_{-3}$ | 9.4 | $0.264_{-5}$ | 8.00 |
| 7 | $0.180_{-4}$ | 8.75 | $0.330_{-6}$ | 8.00 |
| 8 | $0.214_{-5}$ | 8.39 | $0.412_{-7}$ | 8.00 |
| 9 | $0.261_{-6}$ | 8.20 | $0.515_{-8}$ | 8.00 |
| 10 | $0.323_{-7}$ | 8.10 | $0^{2} 644_{-9}$ | 8.00 |

(3.5a) $\mathrm{a}=0.5, \mathrm{~b}=1, \mathrm{c}=1, \mathrm{~d}=1.5, \mathrm{e}=1.5 \quad$ DIRK (4.4)

$$
\tau=0.8 / 2^{i} \quad \tau=0.6 / 2^{i}
$$

Table 4.7. Errors for fourth order methods.

| $\mathbf{i}$ | error | ratio | error | ratio |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | $0.131_{-1}$ |  | $0.880_{-3}$ |  |  |
| 4 | $0.865_{-3}$ | 15.2 | $0.558_{-4}$ | 15.8 |  |
| 5 | $0.545_{-4}$ | 15.9 | $0.350_{-5}$ | 16.0 |  |
| 6 | $0.340_{-5}$ | 16.0 | $0.218_{-6}$ | 16.0 |  |
| Method (3.6) DIRK (4.5) |  |  |  |  |  |
| $\tau=0.8 / 2^{i}$ |  |  |  |  |  |

The above experiments appear to be consistent with the order of the schemes advocated. To test the $L_{0}$-stability we also computed the solution to the following problem.

$$
\begin{equation*}
\frac{\partial u}{\partial t}=\kappa \frac{\partial^{2} u}{\partial x^{2}}+s(x, t)(0<x<1) \times(t>0) \tag{4.2}
\end{equation*}
$$

where $\kappa$ the diffusion coefficient is a constant and the source term $s(x, t)$ is defined by $s(x, t)=s_{1}(x) s_{2}(t)$
where

$$
s_{1}(x)= \begin{cases}0 & 0 \leq x \leq 1 / 4 \\ 1 & 1 / 4<x<3 / 4 \\ 0 & 3 / 4 \leq x \leq 1\end{cases}
$$

and $s_{2}(t)$ represents a time switch which at $\mathrm{t}=0$ is switched on $(=1)$ and switches either on or off $(=0)$ every 1.2 seconds. The numerical solution was continued to $\mathrm{t}=6.2$ using the parameters given. The solution at $\mathrm{x}=0.5$ is given in Fig. 1-6. In all cases $\mathrm{h}=0.05$

In Fig. 1, we see the classical heat response to a switched source. The solution remained essentially invariant under changes in the time step $\tau$. In Fig. 2 the larger value of $\kappa$ produces a much more rapid response to a heat switch. Even with the very large value of $\tau$ the second order method (3.4) produces a solution which represents a rapid response to the switch. As a comparison to indicate the importance of the $L_{0}$-stability, we show in Fig. 3 the results obtained using the Crank Nicolson method $\theta=1 / 2 \alpha=1$ for the same parameters indicated in Fig. 2. The overshoots are apparent.

The same problem was solved using the third order method (3.5) with $\alpha=-\beta$ $=9 / 2$ together with the parameter values $a, b, c \ldots, e$ given by (i) in section 3. In the present piecewise constant heat source the actual parameter values are not pertinent to the order except that $a$ should not be chosen either equal to 0 or 3 as this places integration points exactly on the discontinuity. The results using $a=$ $0.5, b=1, c=2, d=e=1.5$ for $\mathrm{K}=2.5 r=40$ are shown in Fig. 4. A comparison with Fig. 2 might suggest that the third order method has produced a solution which has a less rapid response to the switching of the heat source. This is of course not the case, but rather a consequence of the fact that the solution is printed (and hence graphed) only at intervals of $3 \tau$ compared with intervals of $2 \tau$ for the second order method. The effect of choosing $a=0$ is quite drastic as indicated in Fig. 5.

Finally, the solution obtained using the fourth order algorithm is depicted in Fig. 6. Once again, there is an apparent retarded response to the switching of the heat source which is due to the fact that the solution is printed at intervals of size $4 \tau$.

In all cases, the stable nature of the algorithms is exhibited. For small values of $\tau(\mathrm{r}=5$, say) with small $\kappa(0.5)$, all the algorithms produced identical results to those depicted in Fig. 1. Differences (marginal) between the algorithms appear for the larger values of $\kappa \tau$. With the increasing number of stages, the question of efficiency of the new higher order methods naturally arises.

We see for the second order methods two stages are involved in which 2 factorisations of coefficient matrices and 3 solves are involved per time step. If the coefficient matrix is constant, then, of course we need only carry out the factorisations once initially. For the third order method, three stages are involved in which 3 factorisations of coefficient matrices and 5 solves are involved per time step. The fourth order algorithm involves 4 factorisations and 7 solves (assuming $\alpha=0$ or $\gamma$ $=0$ ). To compare the relative efficiencies of these methods, we assume the algorithms are applied to a one space dimensional heat equation in which case the coefficient matrices are tridiagonal. We can then assert a cost of 2 N operations for a factorisation and 3 N operations per solve; ignoring the cost of matrix/vector
multiplications on the right hand sides of the equations. Consequently, for constant coefficients, we have the relative costs, per time step, given as

2nd order method: 9 N
3rd order method: 15 N operations
4th order methods: 21 N
and ignore the overhead of factorisations; however, see below. In applying these methods, let us assume an error tolerance was set to $0.8_{10-3}$ in which case, from table 4 , we see that if M time steps are needed to reach $t_{\text {max }}$ for the second order scheme, 0.5 M steps are required by the third order scheme and 0.125 M steps are required by the fourth order method. The relative costs are therefore

2nd order: $M^{*} 9 N=9 M N$
3rd order: $0.5^{*} 15 \mathrm{~N}=7.5 M \mathrm{~N}$ operations
4th order: $0.125 M^{*} 21 N=2.625 M N$. The relative efficiencies can be seen in the following ratios

3rd order: 4 th order $=2.8: 1$
2nd order: 4 th order $=3.4: 1$
2nd order: 3 rd order $=1.2: 1$
i.e., the third order method is 2.8 times as expensive as the fourth order method; the second order method is 3.4 times as expensive as the fourth order method and the second order method is 1.2 times as expensive as the third order method. It appears from these simple comparisons that 'order pays'! In comparison, if we now assume variable coefficients, we have to factorize the coefficient matrices at each time step. The relative costs then become:

2nd order: $13 M N$
3rd order: $10.5 M N$ operations
4th order: 3.625 MN
and the relative efficiencies are given by
3rd order: 4 th order $=2.9: 1$
2 nd order: 4 th order $=3.6: 1$
2 nd order: 3 rd order $=1.2: 1$
The actual efficiencies for other partial differential equations (e.g., two space dimensional) may differ slightly from these figures. However, we believe these relative costs indicate the advantages of using the higher order algorithms over the lower order schemes.

## 5. Conclusion

We have generalized the algorithms of Gourlay and Morris (1980) to deal with variable coefficients and inhomogeneous source terms. It appears from the experiments carried out that the algorithms do perform in a fashion predicted by the theory. We have curtailed our investigation of higher order methods as it is our belief that schemes of order four in time should prove adequate for most practical problems. It is our intent to carry out practical (real life) computations with the described methods and to perform meaningful comparisons with other high order time integrators described in the literature. Further, we wish to generalize the current algorithms to other classes of time dependent problems. Hyperbolic systems and equations like the Korteweg de Vries equation and the Burger equation come to mind. As noted earlier, the algorithms covered here apply to any number of space variables provided an efficient (sparse matrix) algorithm exists for solving the associated linear equations (George and Liu 1981). For problems which lend themselves to splitting, there is clearly a need to investigate high order splitting techniques capable of maintaining the order of accuracy developed in the current paper. We hope to have something to report on this in a later paper.

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in revised form 22/05/1983)


Fig. 1. Solution for problem (4.2) to $t=6.0 ; \tau=0.0125(\mathrm{r}=5) ; \varkappa=0.5 ; \theta=0 ; \alpha=2$ : Second order method (3.4).


Fig. 2. Solution for problem (4.2) to $\mathrm{t}=6.0 ; \boldsymbol{\tau}=0.1(\mathrm{r}=40) x=2.5 \theta=0 ; \alpha=2$ : Second order method (3.4).


Fig. 3. Solution for problem (4.2) to $t=6.0 ; \tau=0.1(r=40) x=2.5 \theta=1 / 2 \alpha=1$ (Crank Nicolson method)


Fig. 4. Solution for problem (4.2) to $\mathrm{t}=6.0 ; \tau=0.1(\mathrm{r}=40) x=2.5$; Third order solution (3.5) (i) ( $\mathrm{a}=0.5$ )


Fig. 5. Solution for problem (4.2) to $\mathrm{t}=6.0 ; \tau=0.1(\mathrm{r}=40) x=2.5$; Third order solution (3.5) (i) ( $\mathrm{a}=0.0$ )


Fig. 6. Solution for problem (4.2) to $t=6.0 ; \tau=0.1(r=40) x=2.5$; Fourth order solution (3.6) with $(\alpha, \beta, \gamma, \delta)=(8,40 / 9,0,-32 / 3)$

استكــال طرق المرتبة الأولى في المعامل المتغير والمعـادلات التفـاضليـة الجرئئية غير المتجانسة من نوع التطعى المكافيء
أ ر. جورلاى وج . ل. موريس

اللمكز العلمي لـّركة آى بى ام - ونشستر - انجلترا ؛ وجامعة وترتلو - كندا

تم تعميم طريقـة اويلر الــلاستكـكال العكسي ، والتي وصفها
 المعــامـلات المتغـيرة والمعـادلات غير المتجــانســة من النـوع المكافيء . يناقش البحث أيضاً طرق الرتب الثانية والثالثة والرابعة

