TR/03/83 March 1983

A family of difference schemes for fourth order parabolic partial differential equations.

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ABSTRACT

A family of methods is developed for the numerical solution of fourth order parabolic partial differential equations in one- and two-space variables. The methods are seen to evolve from multiderivative methods for second order ordinary differential equations.

The methods are tested on three model problems, with constant coefficients and variable coefficients, which have appeared in the literature.

1. ONE SPACE DIMENSION

1.1 Introduction

The fourth order parabolic partial differential equation in one space variable given by

$$\frac{\partial^2 u}{\partial t^2} + \mu \frac{\partial^4 u}{\partial x^4} = 0; \quad \mu > 0, \ 0 < x < x, \ t > 0 \tag{1}$$

arises in the study of the transverse vibrations of a uniform flexible beam (see, for example, Gorman [11]). The term μ is the ratio of the flexural rigidity of the beam to its mass per unit length.

The initial conditions associated with (1) are of the form

$$u(x,0) = g_0(x) \ ; \ 0 \le x \le x, \tag{2}$$

$$\frac{\partial u}{\partial t}(x,0) = g_1(x) \ ; \ 0 \le x \le x, \tag{3}$$

and the boundary conditions are given by

$$u(0,t)\text{-}f_0 \ , \quad u(x,t)=f_1; \ t > 0 \tag{4}$$

$$\frac{\partial^2 u}{\partial x^2}(0,t) = p_0, \frac{\partial^2 u}{\partial x^2}(x,t) = p_1 : t > 0 \tag{5}$$

In (2), (3) the functions g_0 (x), g_1 (x) are continuous and in (4), (5) the terms f_0 ,f_1 ,p_0 ,p_1 are real constants.

To compute the solution of (1) with (2), (3), (4), (5), explicit and implicit finite difference schemes have been proposed by Albrecht [1], Collatz [3], Conte [4], Conte and Royster [5], and Crandall [6]. Evans [9] derived finite difference methods by first writing (1) as two simultaneous second order parabolic partial differential equations (see also Du Fort and Frankel [8], and Richtmyer [16]). Explicit and implicit finite difference methods based on the semi-explicit method of Lees [14] and the high order method of Douglas [7] for second order parabolic equations, have been formulated for the numerical solution of (1) with (2), (3), (4), (5) by Fairweather and Gourlay [10].

The explicit method of Collatz [3] frequently needs a large number of time steps to compute the solution in view of the stability restriction on

the method. The difference scheme given by Albrecht [1] overcomes the stability problem but uses the value of the solution at four time levels to compute the solution at a fifth time level, hence requiring a complicated starting procedure. The work of Fairweather and Gourlay [10] gives superior numerical results to the methods of Evans [9] and Richtmyer [16], but more CPU time is required.

In the present paper a family of novel finite difference schemes is developed for the numerical solution of (1) with (2), (3), (4), (5); a related procedure was adopted by Lawson and Morris [13] for second order parabolic equations, by Khaliq and Twizell [12] for first hyperbolic equations and by Twizell [17] for second order hyperbolic equations. The methods developed are shown to have high accuracy and good stability properties and are tested on problems discussed in the literature by Andrade and McKee [2] and Fairweather and Gourlay [10].

1.2 A recurrence relation

The interval $0 \le x \le X$ will be divided into N+1 subintervals each of width h so that (N+1)h = X and the time variable t is discretized in steps of length ℓ. The open region R =[0 < x < X] × [t > 0] and its boundary ∂R consisting of the lines x = 0, x = X, t = 0 are thus covered by a rectangular mesh, the mesh points having coordinates (mh,nℓ) where m = 0,1,...,N+1 and n = 0,1,2,... . The theoretical solution of a difference scheme approximating (1) will be denoted by U_m^n at the mesh point (mh,nℓ).

Superimposing this grid, and assuming that u is sufficiently often differentiable, allows the space derivative in (1) to be approximated by the finite difference replacement

$$\frac{\partial^4 u}{\partial x^4} = h^{-4}\{u(x-2h,t) - 4u(x-h,t) + 6u(x,t) - 4u(x+h,t) + u(x+2h,t)\} + 0(h^4) \qquad (6)$$

for x = mh (m = 1,2,...,N). For m = 1 and m = N, equation (6) introduces the points (-h,t) and (X+h,t) at time t, which are outside the region R.

However, the values of u at these points may be written in terms of function values in R and on R by using (4), (5).

In (5), $\partial^2 u/\partial x^2$ is approximated by the usual second order replacement; this gives

$$\frac{\partial^2 u}{\partial x^2} = h^{-2}\{u(-h,t) - 2u(0,t) + u(h,t)\} + 0(h^2) \tag{7}$$

at the boundary points (0,t) and

$$\frac{\partial^2 u}{\partial x^2} = h^{-2}\{u(X-h,t) - 2u(x,t) + u(X+h,t)\} + 0(h^2) \tag{8}$$

at the boundary points (X,t). Using (4), (5), equations (7), (8) give

$$u(-h,t) = -u(h,t) + 2f_0 + h^2 p_0 + O(h^4), \tag{9}$$

$$u(X+h,t) = -u(X-h,t) + 2f_1 + h^2 p_1 + O(h^4), \tag{10}$$

respectively, and it is these expressions which will be used when (6) is used with x = h and x = (N-1)h.

Consider now the time level $t = n\ell$ and apply (1) with (6) to the N mesh points at this time level. This leads to the system of second order ordinary differential equations given by

$$\frac{d^2 \underset{\sim}{u}}{dt^2} = \mu a \underset{\sim}{u}(t) - \mu \underset{\sim}{w}, \tag{11}$$

where $\underset{\sim}{U}(t) = [U_1(t), U_2(t), \ldots, U_n(t)]^T$, T denoting transpose, is the vector of computed solutions at the N mesh points at time t, A is the square matrix of order N given by

$$A = h^{-4}\begin{bmatrix} 5 & -4 & 1 & & & & \\ -4 & 6 & -4 & 1 & & 0 & \\ 1 & -4 & 6 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 6 & -4 & 1 \\ & 0 & & 1 & -4 & 6 & -4 \\ & & & & 1 & -4 & 5 \end{bmatrix} \tag{12}$$

with eigenvalues

$$\lambda_s = 16h^{-4}\sin^4\left[s\pi/\{2(N+1)\}\right],\quad s = 1,2,...,N \tag{13}$$

and $\underset{\sim}{w}$ is the vector of boundary values of order N given by

$$\underset{\sim}{w} = h^{-4}\,[h^2p_0 - 2f_0\ ,\ f_0\ ,\ 0,...,0\ ,\ f_1\ ,\ h^2\ p_1 - 2f_1]^T\ . \tag{14}$$

Solving (11) subject to the initial conditions (2), (3) gives the analytical solution

$$\begin{aligned}\underset{\sim}{u}(t) = -A^{-1}\underset{\sim}{w} + \frac{1}{2}\exp(i\nu tB)\left\{\underset{\sim}{g}_0 + (i\nu B)^{-1}\underset{\sim}{g}_1 + A^{-1}\underset{\sim}{w}\right\}\\ + \frac{1}{2}\exp(-i\nu tB)\left\{\underset{\sim}{g}_0 - (i\nu B)^{-1}\underset{\sim}{g}_1 + A^{-1}\underset{\sim}{w}\right\},\end{aligned} \tag{15}$$

in which $i = \sqrt{-1}$, $\nu = \sqrt{\mu}$ and B is a matrix such that $B^2 = A$. It is easy to show that (15) satisfies the recurrence relation

$$\begin{aligned}&\underset{\sim}{U}(t+\ell) - (\exp(i\nu\ell B) + \exp(-i\nu\ell B)\underset{\sim}{U}(t) - \underset{\sim}{U}(t-\ell)\\ &\quad = \{\exp(i\nu\ell B) + \exp(-i\nu\ell B)\}A^{-1}\underset{\sim}{w} - 2A^{-1}\underset{\sim}{w}\end{aligned} \tag{16}$$

with $t = \ell, 2\ell, \ldots$. and it is this relation which will be used in the development of the family of algorithms for solving (1) with (2), (3), (4), (5). In view of the approximants to the matrix exponential functions which will be used in (16), it will not be necessary to compute ν, B or A^{-1} directly.

1.3 Solution at the first time step

It is clear that, using (15) with $t = \ell$ requires knowledge of $\underset{\sim}{U}(\ell)$ which, Unlike $\underset{\sim}{U}(0)$, is not contained explicitly in the initial conditions.

Writing $t = \ell$ in (15) and replacing the matrix exponential functions with their (0,3) Padé approximants leads to

$$\underset{\sim}{U}(\ell) = \left(I - \frac{1}{2}\mu\ell^2 A\right)\underset{\sim}{g}_0 + \ell\left(I - \frac{1}{6}\mu\ell^2 A\right)\underset{\sim}{g}_1 - \frac{1}{2}\mu\ell^2\underset{\sim}{w} + 0(\ell^4), \tag{17}$$

replacing the matrix exponential functions with their (0,5) Padé approximants leads to

$$\begin{aligned}\underset{\sim}{U}(\ell) = (I - \frac{1}{2}\mu\ell^2 A + \ell\frac{1}{24}\mu^2\ell^4 A^2)\underset{\sim}{g}_0 + \ell(I - \frac{1}{6}\mu\ell^2 A + \ell\frac{1}{120}\mu\ell^4 A^2)\underset{\sim}{g}_1\\ -\frac{1}{2}\mu\ell^2(I - \frac{1}{12}\mu\ell^2 A)\underset{\sim}{w} + 0(\ell^6)\end{aligned} \tag{18}$$

and using the (0,7) Padé approximants leads to

$$\begin{aligned}\underset{\sim}{U}(\ell) = (I - \frac{1}{2}\mu\ell^2 A + \ell\frac{1}{24}\mu^2\ell^4 A^2 - \frac{1}{720}\mu^3\ell^6 A^3)\,\underset{\sim}{g}_0 \\ + \ell\left(I - \frac{1}{6}\mu\ell^2 A + \frac{1}{120}\mu^2\ell^4 A^2 - \frac{1}{5040}\mu^3\ell^6 A^3\right)\underset{\sim}{g}_1 \\ - \frac{1}{2}\mu\ell^2\left(I - \frac{1}{12}\mu\ell^2 A + \frac{1}{360}\mu^2\ell^4 A^2\right)\underset{\sim}{w} + 0(\ell^8).\end{aligned} \tag{19}$$

In. problems having time dependent boundary conditions f_0, f_1, p_0, p_1 in (4), (5) are functions of t and the vector $\underset{\sim}{w}$ in (17), (18), (19) is evaluated using $t = \ell$ in the equation

$$\underset{\sim}{w}_t = h^{-4}\left[h^2 p_0(t) - 2f_0(t), f_0(t), 0, \ldots, 0, f_1(t), h^2 p_1(t) - 2f_1(t)\right]^T. \tag{20}$$

The complete algorithm for computing the numerical solution of (1) with (2), (3), (4), (5) may thus be listed as follows:

(i) the starting vector $\underset{\sim}{U}(0) = \underset{\sim}{g}_0$ is obtained from equation (2);

(ii) the starting vector $\underset{\sim}{U}(\ell)$ is obtained using (17), (18) or (19) depending on the required accuracy;

(iii) $\underset{\sim}{U}(t+\ell)$, with $t = \ell,\ 2\ell, \ldots$, is obtained from the recurrence relation (16) in which the matrix exponential functions are replaced by suitable approximants.

It is these matrix functions which will be replaced by Padé approximants in §2; in this way the novel family of methods will evolve.

2. THE NUMERICAL METHODS

2.1 Development and analyses of the novel methods

Using the (1,1) Padé approximants to the matrix exponential functions in (16) leads to a difference scheme written in matrix form as

$$(I + \frac{1}{4}\mu\ell^2 A)\,\underset{\sim}{U}(t+\ell) = (2I - \frac{1}{2}\mu\ell^2 A)\,\underset{\sim}{U}(t) - (I + \frac{1}{4}\mu\ell^2 A)\,\underset{\sim}{U}(t-\ell) - \mu\ell^2\,\underset{\sim}{w} + o(\ell^4); \tag{21}$$

for problems with time dependent boundary conditions this becomes

$$\begin{aligned}(I + \frac{1}{4}\mu\ell^2 A)\,\underset{\sim}{U} + \frac{1}{4}\mu\ell^2\,\underset{\sim}{w}_{t+\ell} \\ = (2I - \frac{1}{2}\mu\ell^2 A)\,\underset{\sim}{U}(t) - \frac{1}{2}\mu\ell^2\,\underset{\sim}{w}_t - (I + \frac{1}{4}\mu\ell^2 A)\,\underset{\sim}{U}(t-\ell) - \frac{1}{4}\mu\ell^2\,\underset{\sim}{w}_{t-\ell} + O(\ell^4).\end{aligned} \tag{22}$$

The principal part of the local truncation error of the method based on the (1,1) Padé approximant is given by

$$\frac{1}{6}\mu h^2\ell^2\frac{\partial^6 u}{\partial x^6} - \frac{1}{6}\ell^4\frac{\partial^4 u}{\partial t^4}. \tag{23}$$

The component $\frac{1}{6}\mu h^2 \ell^2 \frac{\partial^6 u}{\partial x^6}$ of (23) is related to the space discretization and the use of (6) in (1); this component will be present in all methods derived by using Padé approximants to the matrix exponential function in (16). The other component of (23) is related only to the Pade approximant chosen for use in (16). The principal part of the local truncation error of any method arising from the use of the (m,k) Padé approximant in (16) will thus have the form

$$\frac{1}{6}\mu h^2 \ell^2 \frac{\partial^{6u}}{\partial x^6} + C_q \ell^q \frac{\partial^q u}{\partial t^q}, \tag{24}$$

where the C_q (q = m+k+1 for m+k odd, and q = m+k+2 for m+k even) are error constants and were derived by the authors in [18]; these error constants are reproduced in Table I. All Padé approximants except the (0,1), (1,0) approximants lead to consistent methods.

Stability, in the conventional sense of a perturbation of the initial data not growing in magnitude as time increases, is analyzed by recourse to the stability equation of the method.

Noting that the (m,k) Padé approximant to the matrix exponential function $\exp(i\nu\ell B)$ has the form

$$\exp(i\nu\ell B) = [Q_m(i\nu\ell B)]^{-1} P_k(i\nu\ell B) + 0(\ell^{m+k+1}) \tag{25}$$

where P_k, Q_m are polynomials of degrees k, m, respectively, with $P_o(i\nu\ell B) \equiv I$ and $Q_o(i\nu\ell B) = I$ (I is the identity matrix of order N), the stability equation has the form

$$Q_m(i\nu\ell\lambda^{\frac{1}{2}})Q_m(i\nu\ell\lambda^{\frac{1}{2}})\xi^2 - \{P_k(i\nu\ell\lambda^{\frac{1}{2}})Q_m(-i\nu\ell\lambda^{\frac{1}{2}}) + P_k(-i\nu\ell\lambda^{\frac{1}{2}})Q_m(i\nu\ell\lambda^{\frac{1}{2}})\}\xi + Q_m(i\nu\ell\lambda^{\frac{1}{2}})Q_m(-i\nu\ell\lambda^{\frac{1}{2}}) = 0. \tag{26}$$

In (26), λ is an eigenvalue of A and ξ is the amplification factor of the method. The non-Neumann necessary condition for stability $|\xi| \le 1$ hence requires

$$\left|P_k(i\nu\ell\lambda^{\frac{1}{2}})Q_m(-i\nu\ell\lambda^{\frac{1}{2}}) + P_k(-i\nu\ell\lambda^{\frac{1}{2}})Q_m(i\nu\ell\lambda^{\frac{1}{2}})\right| \le 2\left|Q_m(-i\nu\ell\lambda^{\frac{1}{2}})Q_m(-i\nu\ell\lambda^{\frac{1}{2}})\right|. \tag{27}$$

In the case of the method based on the (1,1) Padé approximant, the stability equation is

$$(1+\frac{1}{4}\mu\ell^2\lambda)\xi - (2-\frac{1}{2}\mu\ell^2\lambda)\xi + (1+\frac{1}{4}\mu\ell^2\lambda) = 0 \qquad (28)$$

and it easy to show that $|\xi| \leq 1$ for any $r = \ell/h^2 \geq 0$ since $\mu > 0$, $\lambda > 0$. the scheme is therefore unconditionally stable and hance convergent.

Other Padé approximants are now used in the recurrence relation given by (16). Using the (0,2) Padé approximants the resulting finite difference method for problem with time dependent boundary condition may be written in vector form as

$$\underset{\sim}{U}(t+\ell) = (2I - \mu\ell^2 A)\underset{\sim}{U}(t) - \mu\ell^2 \underset{\sim}{w}_t + u(t-\ell) .$$

This is the explicit scheme of Collatz [3] for which $C_4 = \frac{1}{12}$. This method has an error constant which is the same order as that of (22)and, since it is explicit, it would appear to be a more desirable method to use. It is, however, stable only for $r \leq \frac{1}{2\mu^{\frac{1}{2}}}$ and may thus be used only with small time steps.

Turning now to the (1,2) Padé approximant, its use in (16) yields the method

$$(I+\frac{1}{9}\mu\ell^2 A)\underset{\sim}{U}(t+\ell) + \frac{1}{9}\mu\ell^2 \underset{\sim}{w}_{t+\ell}$$

$$= (2I+\frac{7}{9}\mu\ell^2 A)\underset{\sim}{U}(t) - \frac{7}{9}\mu\ell^2 \underset{\sim}{w}_t - (I+\frac{1}{9}\mu\ell^2 A)\underset{\sim}{U}(t-\ell) - \frac{1}{9}\mu\ell^2 \underset{\sim}{w}_{t-\ell} . \qquad (30)$$

From Table I it is seen that $C_4 = -1/36$, so that method enjoys better accuracy than (22) or (29). It's first drawback is that it is an implicit method; furthermore, its stability eqation

$$(1+\frac{1}{9}\mu\ell^2\lambda)\xi^2 - (2-\frac{7}{9}\mu\ell^2\lambda)\xi + \frac{1}{9}(1+\frac{1}{9}\mu\ell^2\lambda) = 0$$

yields the restriction $\mu\ell^2\lambda \leq 36/5$ which, since $\lambda < 16h^{-4}$, leads to the stability condition $r \leq 3\sqrt{5}/(10\sqrt{\mu})$. Thus, although it may be used with slightly bigger time steps than (29), its gain in accuracy and the fact that it is implicit, do not make this method more attractive than (29), or (22) which, though implicit, is unconditionally stable.

A notable improvement in the accuracy in time is obtained by using the (2,2) Padé approximant to the matrix exponential functions in (16). This approximant gives the method

$$(I+\frac{1}{12}\mu\ell^2 A+\frac{1}{144}\mu^2\ell^4A^2)\underset{\sim}{U}(t+\ell)+(\frac{1}{12}\mu\ell^2 I+\frac{1}{144}\mu^2\ell^2 A)\underset{\sim}{w}_{t+\ell}$$
$$=(2I+\frac{5}{6}\mu\ell^2 A+\frac{1}{72}\mu^2\ell^4A^2)\underset{\sim}{U}(t)-(\frac{5}{6}\mu\ell^2 I+\frac{1}{72}\mu^2\ell^4 A)\underset{\sim}{w}_{t}$$
$$-\ (I+\frac{1}{12}\mu\ell^2 A+\frac{1}{144}\mu^2\ell^4A^2)\underset{\sim}{U}(t-\ell)-(\frac{1}{12}\mu\ell^2 I+\frac{1}{144}\mu^2\ell^4 A)\underset{\sim}{w}_{t-\ell} \qquad (31)$$

for which $C_6 = \frac{1}{360}$ (from Table I). The stability equation is

$$(1+\frac{1}{12}\mu\ell^2\lambda+\frac{1}{144}\mu^2\ell^4\lambda^2)\xi^2-(2-\frac{5}{6}\mu\ell^2\lambda+\frac{1}{72}\mu^2\ell^4\lambda^2)\xi+(1+\frac{1}{12}\mu\ell^2\lambda+\frac{1}{144}\mu^2\ell^4\lambda^2)=0$$

from which it is easily verified that the method is unconditionally stable.

Squaring the matrix A involves an increase in the number of mesh points at each time level used in the computation. This notion of using a greater number of points at each time level was used by the authors for first order hyperbolic equations in [12] and by Twizell [17] for second order hyperbolic equations ; Mitchell and Griffiths[15] discussed the concept briefly for second order parabolic equations.

The same order of accuracy in time may be achieved by deleting the terms in A^2 from (31); this gives

$$(I+\frac{1}{12}\mu\ell^2 A)\underset{\sim}{U}(t+\ell)+\frac{1}{12}\mu\ell^2\underset{\sim}{w}_{t+\ell}$$
$$=(2I+\frac{5}{6}\mu\ell^2 A)\underset{\sim}{U}(t)-\frac{5}{6}\mu\ell^2\underset{\sim}{w}_{t}-(I+\frac{1}{12}\mu\ell^2 A)\underset{\sim}{U}(t-\ell)-\frac{1}{12}\mu\ell^2 A)\underset{\sim}{w}_{t-\ell} \qquad (31a)$$

for which $C_6 = {}^{-1}/240$. Equation (31a) is, in fact, an application of Numerov's linear multistep method for the numerical solution of second order ordinary systems and the finite difference scheme resulting from it for the solution of (1) is stable only for $r \le \{3/8\mu\}^{\frac{1}{2}}$. Equation (31a) is clearly very useful when small time steps may be taken.

The (2, 1) Padé approximant leads to the implicit method

$$(I+\frac{1}{9}\mu\ell^2 A+\frac{1}{36}\mu^2\ell^4A^2)\underset{\sim}{U}(t+\ell)+(\frac{1}{9}\mu\ell^2 I+\frac{1}{36}\mu^2\ell^4 A\ )\underset{\sim}{w}_{(t+\ell)}$$
$$=(2I-\frac{7}{9}\mu\ell^2 A)\underset{\sim}{U}(t)-\frac{7}{9}\mu\ell^2\underset{\sim}{w}_{t}$$
$$-\ (I+\frac{1}{9}\mu\ell^2 A+\frac{1}{36}\mu^2\ell^4A^2)\underset{\sim}{U}(t-\ell)-(\frac{1}{9}\mu\ell^2 I+\frac{1}{36}\mu^2\ell^4 A)\underset{\sim}{w}_{(t-\ell)}. \qquad (32)$$

This method has $C_4 = \frac{1}{36}$ and is unconditionally stable. Its theoretical accuracy near the boundary is not second order in time: however, this does not diminish the overall accuracy of the difference scheme (Mitchell and Griffiths [15;pp.112-116,121-125]). Provided sufficiently small time steps may be taken, it may be advisable to delete the terms in A^2 from (32). The method then becomes identical to (30), which has error constant the same magnitude as (32) and which is obviously more economical than (32) in relation to storage requirements.

Using the (2,0) Padé approximant to the matrix exponential functions in (16) gives the implicit scheme

$$(I+\frac{1}{4}\mu^2\ell^2A^2)U(t+\ell)+\frac{1}{4}\mu^2\ell^4\, A\underset{\sim}{w}_{t-\ell}$$
$$= (2I-\mu^2\ell^2A)\underset{\sim}{U}(t)-\mu\ell^2\underset{\sim}{w}_t-(I+\frac{1}{4}\mu^2\ell^4A^2)\underset{\sim}{U}(t-\ell)-\frac{1}{4}\mu^2\ell^4A\underset{\sim}{w}_{t-\ell} \qquad (33)$$

which has error constant C_4 = '7/12. The method is unconditionally stable but its less favourable error constant and the fact that it requires A^2 , suggest that the method based on the (1,1) Padé approximant is to be preferred. It will be seen in subsection 2.2, however, to give generally better numerical results than (22) for the problems tested.

2.2 Numerical results

In order that the behaviour of the schemes in §2.1 might be observed, they were tested on two problems from the literature, as follows:

Problem 2.1 (Fairweather and Gourlay [10])

$$\frac{\partial^2u}{\partial t^2}+\frac{\partial^4u}{\partial x^4}=0 \quad ; \quad 0 < x < 1$$

with initial conditions

$$u(x,0)=\frac{x}{12}(2x^2-x^3-1) \; ; \quad 0 \le x \le 1,$$

$$\frac{\partial u}{\partial t}(x,0)=0 \quad ; \quad 0 \le x \le 1$$

and boundary conditions

$$u(0,t) = u(1,t) = 0 \quad ; \qquad t > 0 \ ,$$

$$\frac{\partial^2 u}{\partial x^2}(0,t) = \frac{\partial^2 u}{\partial x^2}(1,t) = 0 \quad ; \qquad t > 0 \ ,$$

The theoretical solution of the problem is

$$u(x,t) = \sum_{s=1}^{\infty} a_s \sin \pi x \cos s^2 \pi^2 t$$

where $a_s = -8\sin^2 \frac{1}{2} s\pi/(s^5\pi^5)$. Here, u(x,t) is infinitely, often differentiable with respect to both x and t and the methods developed in §2 may be used.

Following Fairweather and Gourlay [10], the increments h, ℓ were given the values h = 0.05, ℓ = 0.00125 (giving r = $\frac{1}{2}$) and the solution computed for t = 0.02. The errors using the methods based on the (1,1), (2,0), (2,1), (2,2) Padé approximants are shown in Table II for x = 0.1(0.1)0.5, the results for x = 0.6(0.1)0.9 being symmetrical to those for x = 0.4(-0.1)0.1. The increments h, ℓ were also given the values h = 0.05, ℓ = 0.005 (giving r = 2) and h = 0.1, ℓ = 0.02 (giving r = 2). The errors using the same four methods for x = 0.1(0.1)0.5 at time t = 1.0 are shown in Tables III, IV.

Comparison of Tables II, III, IV with Tables I, III of Fairweather and Gourlay [10] shows that the new methods based on the (1,1), (2,0), (2,1) Padé approximants give comparable accuracy to the high order correct method of Douglas (adapted and used in Fairweather and Gourlay [10]) while the new method based on the (2,2) Padé approximant gives better accuracy. All the new methods were found to give much better results than the methods of Evans [9], Richtmyer [16] and the semi-explicit method [10;p.9] because of their superior local trunction errors. The numerical results given by the method based on the (2,2) Padé approximant were found to improve as the mesh ratio r increased. This is due to the fact that the component of the principal part of the local truncation error due to the (2,2) Padé approximant is much smaller than the component due to the space discretization. Thus, the best improvement is obtained using this method with large mesh ratios.

Problem 2.2 (Andrade and McKee [2])
This is a variable coefficient problem and is given by

$$\frac{\partial^2 u}{\partial t^2} + \mu(x,t)\frac{\partial^4 u}{\partial x^4} = 0 \quad ; \quad \mu(x,t) > 0 , \quad \frac{1}{2} < x < 1 , \quad t > 0$$

$$\mu(x,t) = \frac{1}{x} + \frac{x^4}{120}$$

with initial conditions

$$u(x,0) = 0 \quad ; \quad \frac{1}{2} \le x \le 1 ,$$

$$\frac{\partial u}{\partial t}(x,0) = 1 + \frac{x^5}{120} \quad ; \quad \frac{1}{2} \le x \le 1$$

and boundary conditions

$$u(\frac{1}{2},t) = \{1 + (\frac{1}{2})^5/120\} \sin t \quad ; \quad t > 0 ,$$

$$u(1,t) = \{1 + (\frac{1}{120}) \sin t \quad ; \quad t > 0 ,$$

$$\frac{\partial^2 u}{\partial x^2}(\frac{1}{2},t) = \frac{1}{6}(\frac{1}{2})^3 \sin t \quad ; \quad t > 0 ,$$

$$\frac{\partial^2 u}{\partial x^2}(1,t) = \frac{1}{6} \sin t \quad ; \quad t > 0 ,$$

The theoretical solution is

$$u(x,t) = \left(1 + \frac{x^5}{120}\right) \sin t .$$

In order to provide a comparison with Andrade and McKee [2], the maximum absolute relative errors were obtained at time t = 0.01 using

(i) h = 0.05 , ℓ = 0.000125 (80 time steps) giving r = 0.05,
(ii) h = 0.05 , ℓ = 0.00025 (40 time steps) giving r = 0.1,
(iii) h = 0.05 , ℓ = 0.000625 (16 time steps) giving r = 0.25;

the results are given in Table V.

It is clear from Table V that the novel methods maintain the same order of accuracy, and their stability properties, for variable coefficient problems as well as constant coefficient problems (see Mitchell and Griffiths [15]). The novel methods of §2 all show an improvement on the method of Andrade and McKee [2] for this problem. It is noticed that the numerical results reported by Andrade and McKee [2] relating to the usual explicit method for

fourth order parabolic equations can be considerably improved. This explicit method is, in fact, the method based on the (0,2) Padé approximant and is, therefore, a member of the family of methods discussed in the present paper. The numerical results relating to this explicit method are contained in Table V and are actually better than the results obtained by Andrade and McKee [2] for their method (denoted by AM in Table V). The numerical results obtained by the present authors using the (0,2) explicit method are better than those for the method based on the (1,1) Padé approximant. This is in accordance with the magnitudes of the time components of the principal parts of the local truncation errors listed in Table I. None of the three mesh ratios used in the numerical experiments violated the stability criteria of the methods based on the (0,2), (1,2) approximants.

3. TWO SPACE DIMENSIONS

3,1 A recurrence relation

It was seen in §2 that the method based on the (2,2) Padé approximant gives rise to accurate numerical results for problems in one space dimension. It is, therefore, worthwhile developing the method for use with problems in two space dimensions.

To that end, consider the test problem

$$\frac{\partial^2 U}{\partial t^2} + V^4 u = 0 \ , \quad V^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} ; \quad 0 < x, y < L \ , \quad t > 0 \tag{34}$$

with initial conditions

$$u(x,y,0) = g_0(x,y) \quad ; \quad (x,y) \in \Omega \ , \tag{35}$$

$$\frac{\partial u}{\partial t}(x,y,0) = g_1(x,y) \quad ; \quad (x,y) \in \Omega \ , \tag{36}$$

where Ω is the interior of the square bounded by the lines $x = 0$, $y = 0$, $x = L$, $y = L$ and $g_0(x, y)$, $g_1(x, y)$ are continuous functions of x, y; the associated boundary conditions are taken to be of the form

$$u(0,y,t) = u(L,y,t) = 0 \quad ; \quad 0 \le y \le L \ , \quad t > 0 \ , \tag{37}$$

$$u(x,y,t) = u(x,L,t) = 0 \quad ; \quad 0 \le x \le L \ , \quad t > 0 \ , \tag{38}$$

$$\frac{\partial^2 u}{\partial x^2}(x,0,t) = \frac{\partial^2 u}{\partial x^2}(x,L,t) = 0 \quad ; \quad 0 \le x \le L \ , \quad t > 0 \ , \tag{39}$$

$$\frac{\partial^2 u}{\partial x^2}(x,y,t) = \frac{\partial^2 u}{\partial x^2}(L,y,t) = 0 \quad ; \quad 0 \le y \le L \ , \quad t > 0 \ , \tag{40}$$

This problem arises in the transverse vibration of a simply supported uniform square plate with each side of length L.

Both intervals $0 \le x \le L$ and $0 \le y \le L$ are divided into N+1 sub-intervals each of width h, so that $(N+1)h = L$, and the time variable t is incremented in steps of length ℓ. At each time level $t = n\ell$ $(n = 0,1,2,\ldots)$ the square Ω together with its boundary $\partial\Omega$ have been superimposed by a square mesh with N^2 points within Ω and N+2 equally spaced points along each edge of $\partial\Omega$.

The solution u(x, y, t) of (34) is to be determined at each. grid point $(kh,mh,n\ell)$ in Ω x [t>0] where $k, m = 1,2,\ldots,N$ and $n = 0,1,2,\ldots$. The theoretical solution of the novel method, to be based on the (2,2) Padé approximant, at the mesh point $(kh,mh,n\ell)$ will be denoted by $\underset{\sim}{U}^n$; the vector $\underset{\sim}{U}^n$ of such solutions will be ordered in the form

$$\underset{\sim}{U}^n = (U^n_1,\ U^n_{2,1},\ldots,\ U^n_{N,1};\ \ U^n_{1,2},\ U^n_{2,2},\ldots,\ U^n_{N,2};\ldots;\ \ U^n_{1,N},\ \ U^n_{2,N},\ldots,\ U^n_{N,N})^T \tag{41}$$

where T denotes transpose.

Replacing the space derivatives in (34) with the usual central difference replacements, $\nabla^4 u$ becomes

$$\begin{aligned}\nabla^4 u = h^{-4}[&u(x+2h,y,t) + u(x,y+2h,t) + u(x-2h,y,t) + u(x,y-2h,t)\\ &+ 2\{u(x+h,y+h,t) + u(x-h,y+h,t) + u(x-h,y-h,t) + u(x+h,y-h,t)\}\\ &- 8\{u(x+h,y,t) + u(x,y+h,t) + u(x-h,y,t) + u(x,y-h,t)\}\\ &+ 20\,u(x,y,t)] + 0(h^2)\ .\end{aligned} \tag{42}$$

Then, applying (34) with (42) to each of the N^2 interior mesh point in the order indicated by (41), and using the boundary conditions (37), (38)—and (39), (40) to eliminate exterior mesh points as in §2—leads to a system of second order ordinary differential equations of the form

$$\frac{d^2 \underset{\sim}{U}(t)}{dt^2} = -s \underset{\sim}{U}(t) \tag{43}$$

where S is a sparse, square matrix of order N^2 given by

$$s = h^{-4} \begin{bmatrix} C & D & E & & & & \\ D & C & D & E & & & \\ E & D & C & D & E & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & E & D & C & D & E \\ & & & E & D & C & D \end{bmatrix}, \tag{44}$$

and C,D,E are square matrices of order N such that

$$c = \begin{bmatrix} 19 & -8 & 1 & & & & \\ -8 & 20 & -8 & 1 & & 0 & \\ 1 & -8 & 20 & -8 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & & \\ & & 1 & -8 & 20 & -8 & 1 \\ & 0 & & 1 & -8 & 20 & -8 \\ & & & & 1 & -8 & 19 \end{bmatrix},$$

$$D = \begin{bmatrix} -8 & 2 & & & \\ 2 & -8 & 2 & & 0 \\ & \ddots & \ddots & \ddots & \\ & & 2 & -8 & 2 \\ 0 & & & 2 & -8 \end{bmatrix}, \quad E = \begin{bmatrix} 1 & & & & \\ & 1 & & & 0 \\ & & \ddots & & \\ & & & 1 & \\ 0 & & & & 1 \end{bmatrix}.$$

The eigenvalues of S are given by

$$\gamma_{r,s} = 16h^{-4}\{\sin^2 \frac{r\pi}{2(N+1)} + \sin^2 \frac{s\pi}{2(N+1)}\}^2 \quad ; \quad r,s = 1,2,...,N . \tag{45}$$

Solving (43), the solution is seen to satisfy the recurrence relation

$$\underset{\sim}{U}(t+\ell) - \{\exp(i\ell F) + \exp(-i\ell F)\}\underset{\sim}{U}(t) + \underset{\sim}{U}(t+\ell) = \underset{\sim}{0} \tag{46}$$

where $i = +\sqrt{-1}$ and F is a matrix such that $F^2 = S$. The starting vectors $\underset{\sim}{U}(0)$, $\underset{\sim}{U}(\ell)$ are required for (46); $\underset{\sim}{U}(0) = g_0$ is obtained from (35), and $\underset{\sim}{U}(\ell)$ is obtained from (17), (18) or (19) with A replaced by S, $\underset{\sim}{w} \equiv \underset{\sim}{0}$ and $\underset{\sim 0}{g}$ $\underset{\sim 1}{g}$ obtained from (35), (36). For the method based on the (2,2) Padé approximant, which has an $0(\ell^6)$ component in the local truncation error (see Table I), the starting vector $\underset{\sim}{U}(\ell)$ is obtained from (18).

3.2 The novel algorithm and its analysis

Using the (2,2) Padé approximant in (46) leads to the algorithm written in vector form as

$$(I+\frac{1}{12}\ell^2S+\frac{1}{144}\ell^4S^2)\,\underset{\sim}{U}(t+\ell)$$
$$=(2I-\frac{5}{6}\ell^2S+\frac{1}{72}\ell^4S^2)\,\underset{\sim}{U}(t)\;-\;(I+\frac{1}{12}\ell^2S+\frac{1}{144}\ell^4S^2)\,\underset{\sim}{U}(t-\ell)\quad . \tag{47}$$

The principal part of the local truncation error of (46) is

$$\left(\frac{1}{6}\,\ell^2h^2\nabla^6u+\frac{1}{360}\ell^6\frac{\partial^6u}{\partial t^6}\right)^n_{k,m}$$

at the grid point $(kh,mh,n\ell)$ and the stability equation is given by

$$(1+\frac{1}{12}\ell^2\gamma\;+\;\frac{1}{144}\ell^4\gamma^2)\;\xi^2-(2-\frac{5}{6}\ell^2\gamma+\;\frac{1}{72}\ell^4\gamma^2)\;\xi+\;(1+\frac{1}{12}\ell^2\gamma+\frac{1}{144}\ell^4\gamma^2)=0$$

where γ is an eigenvalue of S. The method is thus unconditionally stable, since $\gamma > 0$ from (45).

Implementing the algorithm in the form (46) requires the square of the matrix S. An alternative approach is to use complex arithmetic and to implement the method by using the complex splitting

$$\{\frac{1}{2}(1-i\sqrt{3})\,I\;+\;\frac{1}{12}\ell^2S\}\,\underset{\sim}{U}^*\;=\;\{(\sqrt{21}+5)\,I\;-\;\frac{1}{6}\ell^2S\}\,\underset{\sim}{U}(t)$$
$$\{\frac{1}{2}(1-i\sqrt{3})\,I\;+\;\frac{1}{12}\ell^2S\}\,\underset{\sim}{U}(t+\ell)\;=\;\{\frac{1}{2}(-\sqrt{21}+5)\,I\;-\;\frac{1}{12}\ell^2S\}\,\underset{\sim}{U}^*$$
$$\{\frac{1}{2}(1+i\sqrt{3})I+\frac{1}{12}\ell^2S\}\,\underset{\sim}{U}(t-\ell)\quad . \tag{48}$$

This splitting preserves the accuracy and stability of the algorithm but requires more computer time to implement.

The need to square the matrix S is also obviated by writing (46) in the abbreviated form

$$(I+\frac{1}{12}\ell^2 S)U(t+\ell) - (2I-\frac{5}{6}\ell^2 S)(t) + (I+\frac{1}{12}\ell^2 S)U(t-\ell) = 0 \quad ,$$

which has local truncation error with principal part

$$\left(\frac{1}{6}\ell^2 h^2 \nabla^6 u - \frac{1}{240}\ell^6 \frac{\partial^6 u}{\partial t^6}\right)_{k,m}^n$$

at the mesh point $(kh, mh, n\ell)$ and stability interval $0 < r \leq \frac{1}{4}\sqrt{3}$. This implicit, abbreviated form of the novel method has the same order of accuracy as (46) and may be used with small mesh ratios.

3.3 Numerical results

To examine the behaviour of the new method, it was tested on the following variable coefficient problem given in Andrade and McKee [2].

Problem 3.1

$$\frac{\partial^2 u}{\partial t^2} + a(x,y,t)\ \frac{\partial^4 u}{\partial x^4} + b(x,y,t)\ \frac{\partial^4 u}{\partial y^4} = 0 \ ; \quad 0 < x,y, < 1 \ , \quad t > 0 \ ,$$

where

$$a(x,y,t) = \frac{1}{2\pi^2}\ (1 - \frac{x^2}{2} + \frac{y^2}{8} + \frac{t^2}{8}) \ ,$$

$$b(x,y,t) = \frac{1}{2\pi^2}\ (1 - \frac{x^2}{2} + \frac{y^2}{8} + \frac{t^2}{8}) \ ,$$

with initial conditions

$$u(x,y,0) = 0 \qquad ; \ 0 \leq x,y \leq 1 \ ,$$

$$\frac{\partial u}{\partial t}(x,y,,0) = \pi\ \sin\pi i\ \ \sin\pi i \quad ; \ 0 \leq x,y \leq 1 \ ,$$

and boundary conditions given by (37), (38), (39), (40) with L = 1. The theoretical solution is

$$u(x,y,t) = \sin\pi i\ \ \sin\pi i\ \ \sin\pi i \ .$$

The solution was computed at time t = 0.05 using

(i) h = 0.1 , ℓ = 0.0005 (100 time steps) giving r = 0.05,

(ii) h = 0.1 , ℓ = 0.001 (50 time steps), giving r = 0.1,

(iii) h = 0.1 , ℓ = 0.0025 (20 time steps), giving r = 0.25;

the maximum relative errors at time t = 0.05 are given in Table VI.

The results were determined using the new algorithm in the form (46) and also in its complex factor form (47). The results were the same for the two formulations, but the complex factor form used three times as much CPU time as the real form (46). The matrix S was augmented in an obvious way to accommodate the functions a(x,y,t), b(x,y,t) and to take account of the missing mixed derivative.

The numerical results show that the new algorithm performs well with variable coefficient problems, maintaining the predicted accuracy and stability properties. Like the one dimensional case discussed in §2, the new algorithm shows an improvement over the method of Andrade and McKee [2] for problems in two dimensions.

4. CONCLUSIONS

In this paper, families of numerical methods have been developed for the solution of fourth order parabolic partial differential equations in one- and two-space variables.

In developing the methods, the space derivatives in the differential equations were replaced by the familiar finite difference replacements, thus reducing the partial differential equations to systems of second order ordinary differential equations.

The theoretical solution of each system of second order ordinary differential equations was seen to satisfy a recurrence relation involving matrix exponential functions which were replaced by Padé approximants. In this way, the new methods evolved. Analyses showed the methods to be accurate and to possess good stability properties.

The methods were tested on problems from the literature and were seen to improve on results which had been reported in other papers.

Table I: Error constants C_q for the methods developed in §2

Method (Padé)	q	C_q
(1,1)	4	-1/6
(0,2)	4	1/12
(1,2)	4	-1/36
(2,2)	6	1/360
(2,1)	4	1/36
(2,0)	4	7/12

Table II: Maximum errors at time t = 0.02 for Problem 2.1 with h = 0.05, ℓ = 0.00125, r = $\frac{1}{2}$

Method (Padé)	x 0.1	0.2	0.3	0.4	0.5
(1,1)	0.20(-5)	0.36(-5)	0.60(-5)	-0.77(-5)	-0.33(-5)
(2,0)	0.18(-5)	0.39(-5)	0.38(-5)	-0.30(-5)	-0.16(-5)
(2,1)	0.17(-5)	0.35(-5)	0.53(-5)	-0.43(-5)	-0.10(-5)
(2,2)	0.16(-5)	0.27(-5)	0.49(-5)	-0.42(-5)	-0.29(-5)

Table III: Maximum errors at time t = 1.0 f or Problem 2.1 with h = 0.05, = 0.005, r = 2

Method (Padé)	x 0.1	0.2	0.3	0.4	0.5
(1,1)	-0.18(-3)	-0.26(-3)	-0.24(-3)	-0.16(-3)	-0.12(-3)
(2,0)	-0.17(-3)	-0.24(-3)	-0.18(-3)	-0.45(-4)	-0.23(-4)
(2,1)	-0.55(-4)	-0.11(-3)	-0.17(-3)	-0.12(-3)	-0.84(-4)
(2,2)	-0.59(-4)	-0.13(-4)	-0.18(-4)	-0.26(-4)	-0.32(-4)

Table IV: Maximum errors at time t = 1.0 for Problem 2.1 with h = 0.1, ℓ = 0.02, r = 2

Method (Padé)	x = 0.1	0.2	0.3	0.4	0.5
(1,1)	-0.29(-3)	-0.57(-3)	-0.93(-3)	-0.11(-2)	-0.11(-2)
(2,0)	-0.84(-4)	-0.22(-4)	-0.24(-3)	-0.38(-3)	-0.40(-3)
(2,1)	-0.47(-3)	-0.48(-3)	-0.67(-3)	-0.72(-3)	-0.99(-4)
(2,2)	-0.21(-3)	-0.45(-3)	-0.35(-3)	-0.23(-3)	-0.74(-4)

Table V: Maximum relative error moduli at time t = 0.01 for Problem 2.2

r	Time Steps	Method (1,1)	(0,2)	(1,2)	(2,0)	(2,1)	(2,2)	AM
0.05	80	0.35(-6)	0.33(-6)	0.35(-6)	0.35(-6)	0.33(-6)	0.99(-7)	0.19(-5)
0.1	40	0.34(-6)	0.35(-6)	0.35(-6)	0.34(-6)	0.33(-6)	0.81(-7)	0.72(-6)
0.25	16	0.32(-6)	0.34(-6)	0.39(-6)	0.33(-6)	0.32(-6)	0.69(-7)	0.41(-6)

Table VI: Maximum relative error moduli at time t = 0.05 for Problem 3.1

R	Time Steps	Methods AM	(2,2)
0.05	100	0.27(-5)	0.87(-6)
0.1	50	0.87(-6)	0.73(-6)
0.25	20	0.40(-6)	0.71(-6)

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