The Extrapolation of First Order Methods for Parabolic Partial Differential Equations I

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Abstract: Splitting methods for parabolic partial differential equations based on (1,1) Padé approximations (Crank-Nicolson replacements) are well known to produce poor numerical results when a time discretization is imposed with time steps which are "too large" relative to the spatial discretization. In particular such numerical solutions exhibit an oscillatory behaviour which increases in amplitude with a reduction in the spatial discretization, keeping the time step constant. In contrast, (1,0) Padé approximations (backward-difference, or fully implicit replacements) do not suffer from these drawbacks but are of lower order accuracy. In the present paper, a combination of fully implicit methods is used to attain second order accuracy and to retain the favorable property of the fully implicit scheme. The method is tested on a heat equation in two space dimensions which possesses a discontinuity between the initial and boundary conditions.

1. Introduction

In several recent papers, Lawson and Swayne [2], Smith, Siemieniuch and Gladwell [5], Wood and Lewis [7], attention has been drawn to restrictions on the time discretization in the Crank-Nicolson method when applied to certain problems. To be precise, consider a constant coefficient heat equation in one space variable

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad [0 < x < 2] \times [t > 0] \ , \tag{1.1}$$

subject to: $u(0,t) = u(1,t) = 0$; $u(x,0) = g(x)$,
where $g(x)$ is a given continuous function of x. In particular, we are interested in the situation where $g(0) \neq 0$ and $g(2) \neq 0$ so that a discontinuity exists between the initial function $g(x)$ and the boundary conditions $u(0,t) = 0$ and $u(1,t) = 0$.

Superimposing a uniform grid of step size h on the space variable in the usual way allows the replacement of the second order derivative in eq. (1.1) by, say, the central-difference operator, namely

$$\frac{du}{dt} = \frac{\delta_x^2}{h^2} u(x,t) + O(h^2) \ , \tag{1.2}$$

where $\delta_x^2 u(x,t) \equiv u(x+h,t) + u(x-h,t) - 2u(x,t)$.
Eq. (1.2) is then applied to all interior mesh points to produce a system of ordinary differential equations

$$\frac{d\underset{\sim}{v}}{dt} = A\underset{\sim}{v}(t) \ , \tag{1.3}$$

where $\underset{\sim}{v} = (v_1, v_2, \ldots, v_N)^T$ is an N-vector of the (unknown) approximation to $\underset{\sim}{u}$ and it is assumed that $(N+1)h = 2$. If we solve eq. (1.3) formally we obtain

$$\underset{\sim}{y}(t) = \exp(tA)\underset{\sim}{y}(0) \tag{1.4}$$

where $\underset{\sim}{y}(0) = \underset{\sim}{g}$ is the vector of initial values. Eq. (1.4) may be written in a step wise fashion as

$$\underset{\sim}{y}(t+\tau) = \exp(\tau A)\underset{\sim}{y}(t) \ , \ t = \tau, 2\tau, \ldots \ , \tag{1.5}$$

where τ is a convenient time step.

The matrix A is the usual tridiagonal matrix of order N given by

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & 0 \\ & \ddots & \ddots & \ddots & \\ & & & \ddots & 1 \\ 0 & & & 1 & -2 \end{bmatrix} .$$

To obtain solutions $\underset{\sim}{y}(t+\tau)$, Padé approximations to the function $\exp(\tau A)$ can be used. In particular, if the diagonal (1,1) approximation

$$(I - \tfrac{\tau}{2} A)^{-1}(I + \tfrac{\tau}{2} A) \doteq \exp(\tau A)$$

is used we incur an error of $O(\tau^3)$. This is, of course, just the familiar Crank-Nicolson method

$$\underset{\sim}{y}(t+\tau) = (I - \tfrac{\tau}{2} A)^{-1}(I + \tfrac{\tau}{2} A)\ \underset{\sim}{y}(t) \tag{1.6}$$

or $$(I - \tfrac{\tau}{2} A)\ \underset{\sim}{y}(t+\tau) = (I + \tfrac{\tau}{2} A)\ \underset{\sim}{y}(t) \ .$$

If we assume that the initial function $\underset{\sim}{g}$ is written as a linear combination of the normalized eigenvectors $\underset{\sim}{w}_i$, i=1,2,...,N of A, say

$$\underset{\sim}{g} = \sum_{i=1}^{N} \alpha_i \underset{\sim}{w}_i$$

then the theoretical solution of eq. (1.6) may be written

$$\underset{\sim}{v}(n\tau) = \sum_{i=1}^{N} \alpha_i \left[\frac{(1 + \frac{\tau}{2}\lambda_i)}{(1 - \frac{\tau}{2}\lambda_i)}\right]^n \underset{\sim}{w}_i , \qquad (1.7)$$

where $\{\lambda_i < 0\}$ are the eigenvalues of A given by

$$\lambda_i = \frac{-4}{h^2} \sin^2\left[\frac{i\pi}{2(N+1)}\right] , \; i = 1,2,...,N .$$

Equation (1.7) shows explicitly that there is no stability restriction on τ for the Crank-Nicolson scheme since the growth factor associated with eigenvector $\underset{\sim}{w}_i$ is $(1 - \frac{\tau}{2}\lambda_i)^{-1}(1 + \frac{\tau}{2}\lambda_i)$. This function is less than 1 in modulus for all τ, since all $\lambda_i < 0$.

However, it is easy to see that this function has values close to -1 if $\tau\lambda_i$ is large and negative. This will be the case if h is small for those λ_i corresponding to i = N, N-1, ... since, for example, $\sin^2\left[\frac{N\pi}{2(N+1)}\right] \simeq 1$ and $\lambda_N \simeq \frac{-4}{h^2}$.

Accordingly, one may expect to see components $\alpha_N \underset{\sim}{w}_N$, $\alpha_{N-1}\underset{\sim}{w}_{N-1}$,... of the initial condition preserved at subsequent solution steps, but with alternating sign. For problems with smooth initial data, such an effect may not be noticed. But, for initial conditions with discontinuities such discontinuities are preserved and distorted rather than damped out; large values of α_N, α_{N-1},... characterize discontinuous problems.

Because of this oscillatory behaviour for sufficiently large τ , it is commonly suggested that the time step τ should be restricted so as to prevent oscillatory solutions. This would imply preventing the numerator of the growth factor in eq. (1.7) becoming negative which imposes the condition

$$\tau \leq \frac{-2}{\lambda_i} \qquad i = 1,2,\ldots,N \quad ,$$

which in turn imposes the condition (approximately)

$$\tau \leq \frac{h^2}{2} \tag{1.8}$$

(see [7]). However, we feel that this restriction is not strictly necessary-oscillatory components are permissible provided they decay to zero <u>faster</u> than the decay of the primary components. In particular, the dominant component is damped each time step by the factor $(1 - \frac{\tau}{2}\lambda_1)^{-1}(1 + \frac{\tau}{2}\lambda_1)$. In contrast the last component is damped each time step by the factor $(1 - \frac{\tau}{2}\lambda_N)^{-1}(1 + \frac{\tau}{2}\lambda_N)$. Thus, to ensure that the higher frequency component, be it oscillatory or not, is damped to zero <u>faster</u> than the lowest frequency component we require

$$\left|\frac{1 + \frac{\tau}{2}\lambda_N}{1 - \frac{\tau}{2}\lambda_N}\right| < \left|\frac{1 + \frac{\tau}{2}\lambda_1}{1 - \frac{\tau}{2}\lambda_1}\right| \quad .$$

That is,

$$\frac{-1 - \frac{\tau}{2}\lambda_1}{1 - \frac{\tau}{2}\lambda_1} < \frac{1 + \frac{\tau}{2}\lambda_N}{1 - \frac{\tau}{2}\lambda_N} < \frac{1 + \frac{\tau}{2}\lambda_1}{1 - \frac{\tau}{2}\lambda_1} \quad . \tag{1.9}$$

The right-hand-side inequality in (1.9) is trivially satisfied, whereas the left-hand inequality imposes the restriction

$$\tau < \frac{2h}{\pi} \qquad \text{(approximately)}.$$

Namely, to produce solutions which damp high frequency components at a faster rate than the low frequency components we have a linear relation between τ and h (not second order as is commonly used). This restriction is less severe than that implied by (1.8) but still restricts τ as being small.

If, in contrast to proposing (1,1) Padé approximations to $\exp(\tau A)$ in eq. (1.5), (1,0) Padé approximations are used, then we obtain the familiar implicit, backward-difference scheme

$$(I - \tau A)\underset{\sim}{v}(t + \tau) = \underset{\sim}{v}(t) \ . \qquad (1.10)$$

An analysis of this method indicates that the method is stable for all positive τ. Furthermore, the growth factor is always positive so that no oscillatory behaviour can arise. However, eq. (1.10) is only first order accurate in time, and is therefore likely to require a smaller τ to attain the same accuracy as that attainable by the Crank-Nicolson method, for smooth initial data. To circumvent this problem, Lawson and Swayne [2] introduce a (2,1) rational approximation which has second order accuracy and which is unconditionally stable. The actual format of their method is given by

$$\begin{aligned} (I - b\tau A)\ \underset{\sim}{v}^* &= \underset{\sim}{v}(t) \\ (I - b\tau A)\ \underset{\sim}{v}^{**} &= \underset{\sim}{v}^* \end{aligned} \qquad (1.11)$$

$$\underset{\sim}{y}(t + \tau) = (\sqrt{2} + 1)\ \underset{\sim}{y}^{**} - \sqrt{2}\ \underset{\sim}{y}^{*},$$

where $b = 1 - \frac{1}{2}\sqrt{2}$ and $\underset{\sim}{y}^{*}$ and $\underset{\sim}{y}^{**}$ are intermediate vectors.

This method works well in practice on the type of discontinuous problems of interest here and requires roughly double the amount of work per step as the Crank-Nicolson method. The method (1.11), however, does not lend itself to generalizations to higher space dimensions. For this reason, we propose an alternative algorithm which generalizes in a natural way to several space variables.

In section 2 we introduce the novel algorithm for a constant coefficient equation in one space variable and test the method on a problem of the type described by eq. (1.1). In section 3 we generalize the method to two space variables and consider a two dimensional analogue of eq. (1.1). The generalizations to higher space dimensions are described briefly in the concluding section 4.

2. Extrapolation of the Fully Implicit Scheme

Consider eq. (1.8) written over a time interval 2τ so that

$$\underset{\sim}{y}(t + 2\tau) = (I - 2\tau A)^{-1} \underset{\sim}{y}(t). \tag{2.1}$$

Alternately if eq. (1.8) is applied twice we have

$$\underset{\sim}{y}(t + 2\tau) = (I - \tau A)^{-1} (I - \tau A)^{-1} \underset{\sim}{y}(t). \tag{2.2}$$

Consequently eqs. (2.1) and (2.2) are two alternative backward-difference schemes for computing the solution at time $t + 2\tau$. The expansion of the matrix inverse in eq. (2.1) produces

$$\underset{\sim}{y}(t + 2\tau) = (I + 2\tau A + 4\tau^2 A^2) \underset{\sim}{y}(t) + 0 (t^3). \tag{2.3}$$

In contrast an expansion of eq. (2.2) produces

$$\underset{\sim}{y}(t + 2\tau) = (I + 2\tau A + 3\tau^2 A^2) \underset{\sim}{y}(t) + 0 (\tau^3). \tag{2.4}$$

The Maclaurin expansion of $\exp(2\tau A)$ produces

$$\underset{\sim}{y}(t + 2\tau) = (I + 2\tau A + 2\tau^2 A^2) \underset{\sim}{y}(t) + 0 (\tau^3), \tag{2.5}$$

so that we see that neither eq. (2.3) nor eq. (2.4) is $0(\tau^2)$ accurate. However, if we combine the expansions in eqs. (2.3) and (2.4) by taking 2* eq. (2.4) and subtracting eq. (2.3) we find

$$\underset{\sim}{y}(t + 2\tau) = (I + 2\tau A + 2\tau^2 A^2) \underset{\sim}{y}(t) + 0 (\tau^3).$$

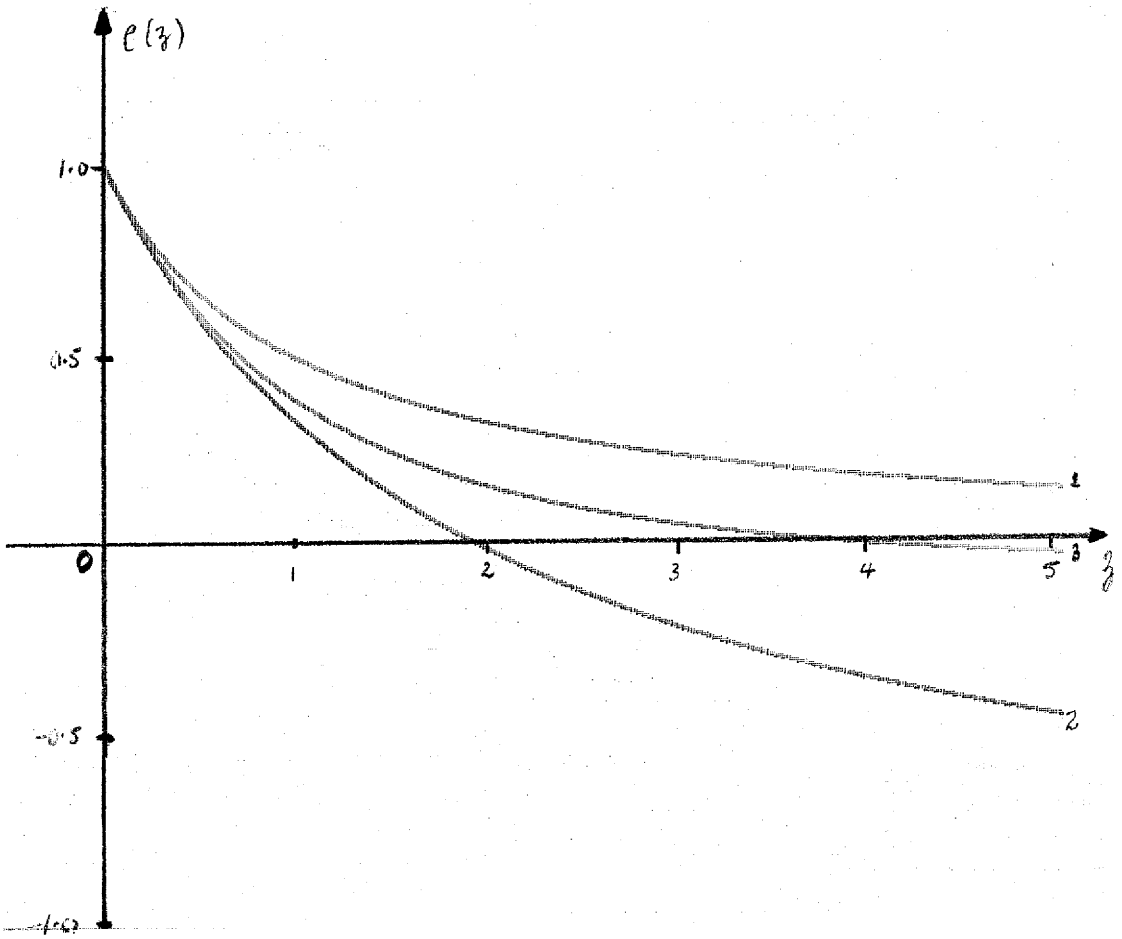

Figure 1. Amplification factors for the schemes: Backward-Difference (1), Crank-Nicolson (2), and Extrapolation (3).

Consequently this suggests the algorithm:

$$\begin{aligned} \underset{\sim}{y}^{(1)}(t + 2\tau) &= (I - 2\tau A)^{-1}\, \underset{\sim}{y}(t) \\ \underset{\sim}{y}^{(2)}(t + 2\tau) &= (I - \tau A)^{-1}(I - \tau A)^{-1}\, \underset{\sim}{y}(t) \qquad (2.6) \\ \underset{\sim}{y}(t + 2\tau) &= 2\underset{\sim}{y}^{(2)} - \underset{\sim}{y}^{(1)}. \end{aligned}$$

$\underset{\sim}{y}(t + 2\tau)$ is now a second order approximation to the solution $\underset{\sim}{y}(t + 2\tau)$.

An analysis of the stability of the algorithm defined by eq. (2.6) indicates that the method is stable for all positive τ. In figure 1 we have plotted the amplification factors $\rho(z)$ against z for the backward-difference scheme, (graph 1), the Crank-Nicolson method (graph 2) and the novel extrapolated scheme (graph 3). As can be seen, the asymptotic behaviour of the backward-difference scheme produces a growth factor which tends to zero, monotonically. In contrast the extrapolated scheme has a growth factor which leads to zero asymptotically but has a small negative value for $z > 2(1 + \sqrt{2})$. This implies that small oscillatious could theoretically appear but these should be damped with increasing t. The Crank-Nicolson method has a growth factor which tends asymptotically to -1. Consequently errors which occur during the computation will tend to be damped at a considerably lower rate than the rate at which the theoretical solution tends to zero.

To show the behaviour of these schemes, we solved the problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad [0 < x < 2] \times (t > 0),$$

$$u(x,t) = 1,$$

$$u(0,t) = u(2,t) = 0.$$

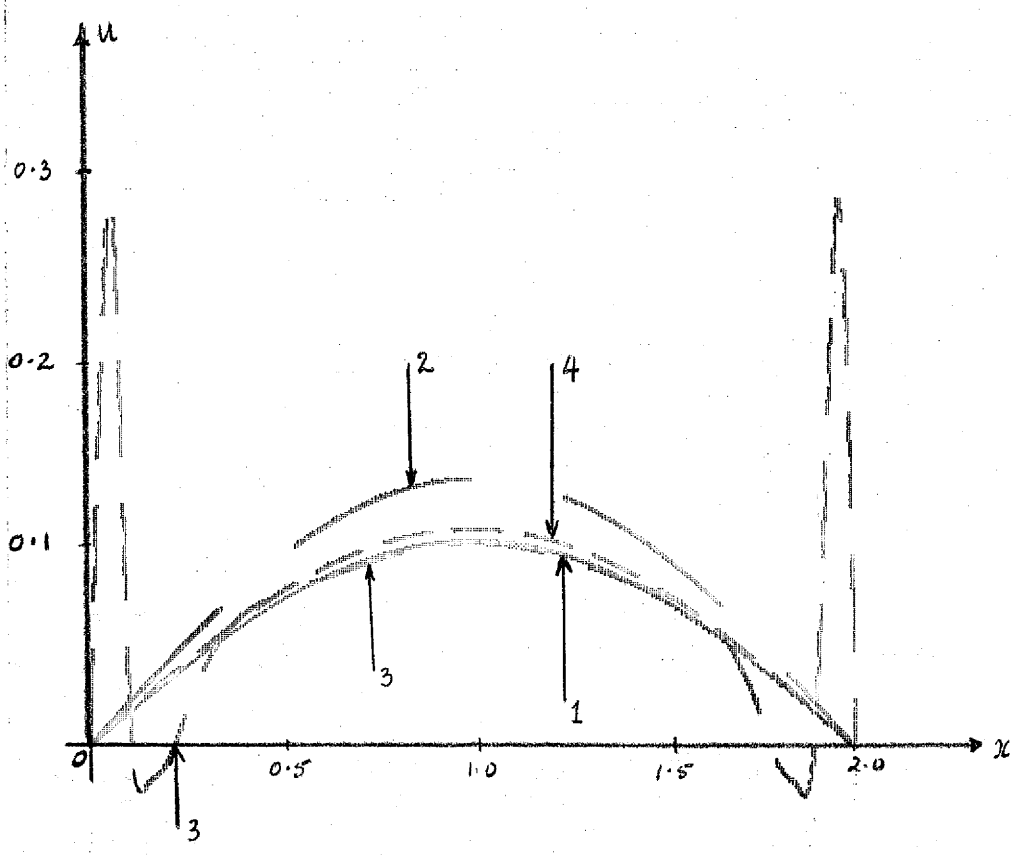

Figure 2. Model problem solutions with $h = 0.05$ and $\tau = 0.1$: Fourier sum (1), Backward-Difference (2), Crank-Nicolson (3), and Extrapolation (4).

which has a theoretical solution

$$u(x,t) = \sum_{n=1}^{\infty} [1-(-1)^n] \frac{4}{n\pi} \sin(\frac{n\pi x}{2}) \exp(\frac{-n^2\pi^2 t}{4})$$

The solutions obtained for $h = 0.05$ are depicted in figure 2, In the figure , curve 1 is the theoretical solution, curve 2 is the backward-difference solution eq. (1.8), curve 3 is the Crank-Nicolson solution eq. (1.6) and curve 4 is the extrapolated scheme solution, eq. (2.6). In all cases a value of the time step $\tau = 0.1$ was used.

As can be seen from the figures, the Crank-Nicolson scheme is accurate in the interior of the region but has a large residual error near the boundary. If h were to be reduced, keeping τ constant, the amplitude of this residual error would increase. The backward-difference scheme portrays a smooth behaviour for all n but is inaccurate uniformly across the interval. In contrast the novel scheme has a smooth representation of the theoretical solution over the whole region, is considerably more accurate than the backward-difference scheme and is comparable with the Crank-Nicolson scheme in the interior of the region. We have tabulated in Table 1 the maximum errors (the difference between the theoretical solution and computed solution) for three values of h for each of the three methods. Note that the actual solution at $x = 1$ and $t = 1$ is about 0.1.

Method	$\tau = 0.1$			$\tau = 0.01$		
	h=0.1	h=0.05	h=0.025	h=0.1	h=0.05	h=0.025
Backward-Difference	.33E-01	.32E-01	.32E-01	.36E-02	.34E-02	.33E-02
Crank-Nicolson	.56E-01	.28E+00	.55E+00	.40E-03	.10E-03	.10E-03
Extrapolation Method	.63E-02	.61E-02	.60E-02	.50E-03	.20E-03	.20E-03

Table 1. Errors in solving the model problem at t = 1.

For $\tau = 0.1$ the backward-difference method incurs an error of approximately 30%. In contrast the extrapolated scheme is more accurate incurring only about 6% error. The Crank-Nicolson method incurs the maximum error at points adjacent to the boundary. Relative to the maximum value of the solution (at x = 1.0) this error is approximately ½, 2½ and 5 times (!) the solution for h = 0.1, 0.05 and h = 0.025 respectively.

Also in Table 1 we have tabulated the errors for a smaller value of $\tau = 0.01$. It may be seen that the errors are uniformly smaller. The results for h = 0.05 and h = 0.025 demonstrate that the error coefficient of the Crank-Nicolson scheme is just one half that of the novel scheme (as could be shown by expanding equations 2.3 - 2.5). Also, it should be noted that these Crank-Nicolson solutions all violate $\tau < \frac{h^2}{2}$ but satisfy $\tau < \frac{2h}{\pi}$, confirming our previous analysis.

3. The Extrapolated Method in Two Space Variables

Consider the simple heat equation in two space variables

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}, \qquad 0 < x,y < 2, \qquad (3.1)$$

subject to a given $u(x,y,0) = g(x,y)$, and given homogeneous Dirichlet boundary conditions ($u \equiv 0$) on the boundary $\delta\Omega$ of the square. Assume further that $g(x,y) \not\equiv 0$ for $(x,y) \in \delta\Omega$.

Following section 1 a system of ordinary differential equations equations

$$\frac{d\underset{\sim}{v}}{dt} = A\underset{\sim}{v}(t) \qquad (3.2)$$

arises when the spatial derivations in eq. (3.1) are replaced by differences. Assuming a uniform discretization of size h in both x and y directions, and that $h = 2/(N+1)$, we have a vector $\underset{\sim}{v}$ of unknowns of dimension N^2. The matrix A is $N^2 \times N^2$.

As before, the solution to eq. (3.2) is given by

$$\underset{\sim}{v}(t+\tau) = \exp(\tau A)\underset{\sim}{v}(t) \qquad (3.3)$$

$$\underset{\sim}{v}(0) = \underset{\sim}{g}, \quad \text{the vector of initial values.}$$

The backward-difference approximation in two space variables is obtained by using (1,0) Padé approximations to the $\exp(\tau A)$ in eq. (3.3). However, this now involves solving systems of equations whose coefficient matrix has band width $2N$, only a few of whose elements per row are nonzero. Consequently, the matrix A is <u>split</u> into constituent matrices A_1 and A_2 such that $A = A_1 + A_2$.

Hence, equation (3.3) becomes

$$\underset{\sim}{v}(t+\tau) = \exp[\tau(A_1 + A_2)]\ \underset{\sim}{v}(t) \tag{3.4}$$

which may be approximated by

$$\underset{\sim}{v}(t+\tau) = \exp(\tau A_2)\exp(\tau A_1)\ \underset{\sim}{v}(t), \tag{3.5}$$

incurring an error $O(\tau^2)$. For each of these exponentials, (1,0) Padé approximations are proposed and there then results a split form of the totally implicit scheme, given by

$$\begin{aligned}(I - \tau A_1)\underset{\sim}{v}^* &= \underset{\sim}{v}(t) \\ (I - \tau A_2)v(t + \tau) &= \underset{\sim}{v}^*\end{aligned} \tag{3.6}$$

where $\underset{\sim}{v}^*$ is an intermediate vector. As is well known, this two step procedure has the advantage of being easily solved, when the components of the second step of eq. (3.6) are reordered. In particular, if the second order derivatives in eq. (3.1) are replaced by central differences then A is an $N^2 \times N^2$ matrix which has 5 nonzero bands. The matrices A_2 and A_1 may be written as tensor products of $N \times N$ tridiagonal matrices so that eq. (3.6) may be solved by implementing sequences of tridiagonal matrix solvers.

The algorithm is first order accurate in time, unconditionally stable and has a growth factor which tends asymptotically to zero. Hence no residual boundary errors will be exhibited.

In contrast to eq. (3.5), eq. (3.4) may be approximated to $O(\tau^2)$ accuracy by

$$\underset{\sim}{v}(t+\tau) = \exp(\tfrac{\tau}{2} A_1)\, \exp(\tau A_2)\, \exp(\tfrac{\tau}{2} A_1) v(t).$$

Hence, on proposing in turn (1,0), (1,1) and (0,1) Padé approximations, the Peaceman - Rachford scheme [3]

$$(I - \tfrac{\tau}{2} A_2)\underset{\sim}{v}^* = (I + \tfrac{\tau}{2} A_1)\underset{\sim}{v}(t)$$

$$(I - \tfrac{\tau}{2} A_1)\underset{\sim}{v}(t+\tau) = (I + \tfrac{\tau}{2} A_2)\underset{\sim}{v}^* \qquad (3.7)$$

is obtained. An efficient implementation of this algorithm is reported in [1].

This algorithm is second order accurate in time, unconditionally stable but has essentially the same restriction on the time step τ as was the case for the Crank Nicolson method.

To obtain the two dimensional analog of the extrapolated scheme described in the previous section,we clearly do not want to take as a basis the backward difference scheme defined in terms of A. Rather, we propose using eq. (3.6).

Consider this equation written over two time steps as

$$(I - \tau A_1)\underset{\sim}{v}^* = \underset{\sim}{v}(t)$$

$$(I - \tau A_2)\underset{\sim}{v}(t+\tau) = \underset{\sim}{v}^*$$

$$(I - \tau A_2)\underset{\sim}{v}^{**} = \underset{\sim}{v}(t+\tau)$$

$$(I - \tau A_1)\underset{\sim}{v}^{(0)}(t+2\tau) = \underset{\sim}{v}^{**}. \qquad (3.8)$$

Equation (3.8) is a symmetrized application of the method (3.6) in that the order in which the matrices A_1 and A_2 appear in the tridiagonal solutions alternates. Eliminating the intermediate vectors in eq. (3.8) and expanding the resulting inverses to $O(\tau^2)$ we find

$$\underset{\sim}{v}^{(0)}(t+2\tau) = [I+2\tau(A_1+A_2)+\tau^2(3A_1^2+3A_2^2+2A_1A_2+2A_2A_1)]\underset{\sim}{v}(t)+O(\tau^3) \tag{3.9}$$

The Maclaurin expansion of eq. (3.4) is

$$\underset{\sim}{v}(t+2\tau) = [I+2\tau(A_1+A_2)+2\tau^2(A_1^2+A_2^2+A_1A_2+A_2A_1)]\underset{\sim}{v}(t)+O(\tau^3) \tag{3.10}$$

so that eq. (3.8) is $O(\tau)$ accurate.

Now consider, in addition to eq. (3.8), defining

$$\underset{\sim}{v}^{(1)}(t+2\tau) = (I - 2\tau A_1)^{-1}(I - 2\tau A_2)^{-1}\underset{\sim}{v}(t) \tag{3.11}$$

and

$$\underset{\sim}{v}^{(2)}(t+2\tau) = (I - 2\tau A_2)^{-1}(I - 2\tau A_1)^{-1}\underset{\sim}{v}(t) \tag{3.12}$$

Expanding the inverses in eqs. (3.11) and (3.12) to $O(\tau^2)$ we find

$$\underset{\sim}{v}^{(1)}(t+2\tau) = [I+2\tau(A_1+A_2)+4\tau^2(A_1^2+A_1A_2+A_2^2)]\underset{\sim}{v}(t)+O(\tau^3) \tag{3.13}$$

$$\underset{\sim}{v}^{(2)}(t+2\tau) = [I+2\tau(A_1+A_2)+4\tau^2(A_1^2+A_2A_1+A_2^2)]\underset{\sim}{v}(t)+O(\tau^3) \tag{3.14}$$

Now consider the linear combination of the three first order schemes (3.8), (3.11) and (3.12), defined by

$$\underset{\sim}{v}(t+2\tau) = 2\underset{\sim}{v}^{(0)} - \frac{1}{2}(\underset{\sim}{v}^{(1)} + \underset{\sim}{v}^{(2)}) \qquad (3.15)$$

Applying this weighting to the expansions in eqs. (3.9), (3.13) and (3.14) and comparing with eq. (3.10) we find that $\underset{\sim}{v}(t+2\tau)$ defined by eq. (3.15) is second order accurate. That is, we have extrapolated the first order methods to achieve second order accuracy.

A simple stability analysis indicates that this novel method is unconditionally stable and possesses an asymptotic growth factor similar to the one dimensional analogue.

The novel algorithm requires 4 tridiagonal solutions per time step. This compares with two required by the Peaceman-Rachford method. However, the time step τ is unrestricted in the novel scheme and consequently we may take time steps (at least) twice as large as the Peaceman-Rachford scheme, for a given h.

To demonstrate the numerical properties of the novel algorithm we computed the solution to the problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad , \qquad 0 < x,y < 2, \qquad (3.16)$$

subject to $u(x,y,0) = \sin \frac{\pi}{2} y, \quad 0 \leq x,y \leq 2;$

and $u(x,y,0) = 0 \quad , \qquad \forall (x.y) \in \delta\Omega \quad , \quad \forall t > 0.$

The initial function is depicted in figure 3. The Fourier solution of this problem is easily found to be

$$u(x,y,t) = \sin \frac{\pi}{2} y \sum_{n=1}^{\infty} [1-(-1)^n] \frac{4}{n\pi} \sin(\frac{n\pi x}{2}) \exp(\frac{-\pi^2}{4}(n^2+1)t). \qquad (3.17)$$

The solution was computed using the backward-difference scheme (3.8), the Peaceman Rachford scheme (3.7) and the novel algorithm { (3.8), (3.11), (3.12) and (3.15)} using a fixed time step $\tau = 0.1$. The theoretical solution at $t = 1.0$ is depicted in figure 4. The backward-difference scheme (3.8) produced results depicted in figure 5 using $h = 0.05$. The general appearance of the solution is good although the inaccuracy due to the first order accuracy of the scheme is apparent as shown by the results in table 2.

Figure 6 shows the results obtained by the Peaceman Rachford scheme using $h = 0.05$.

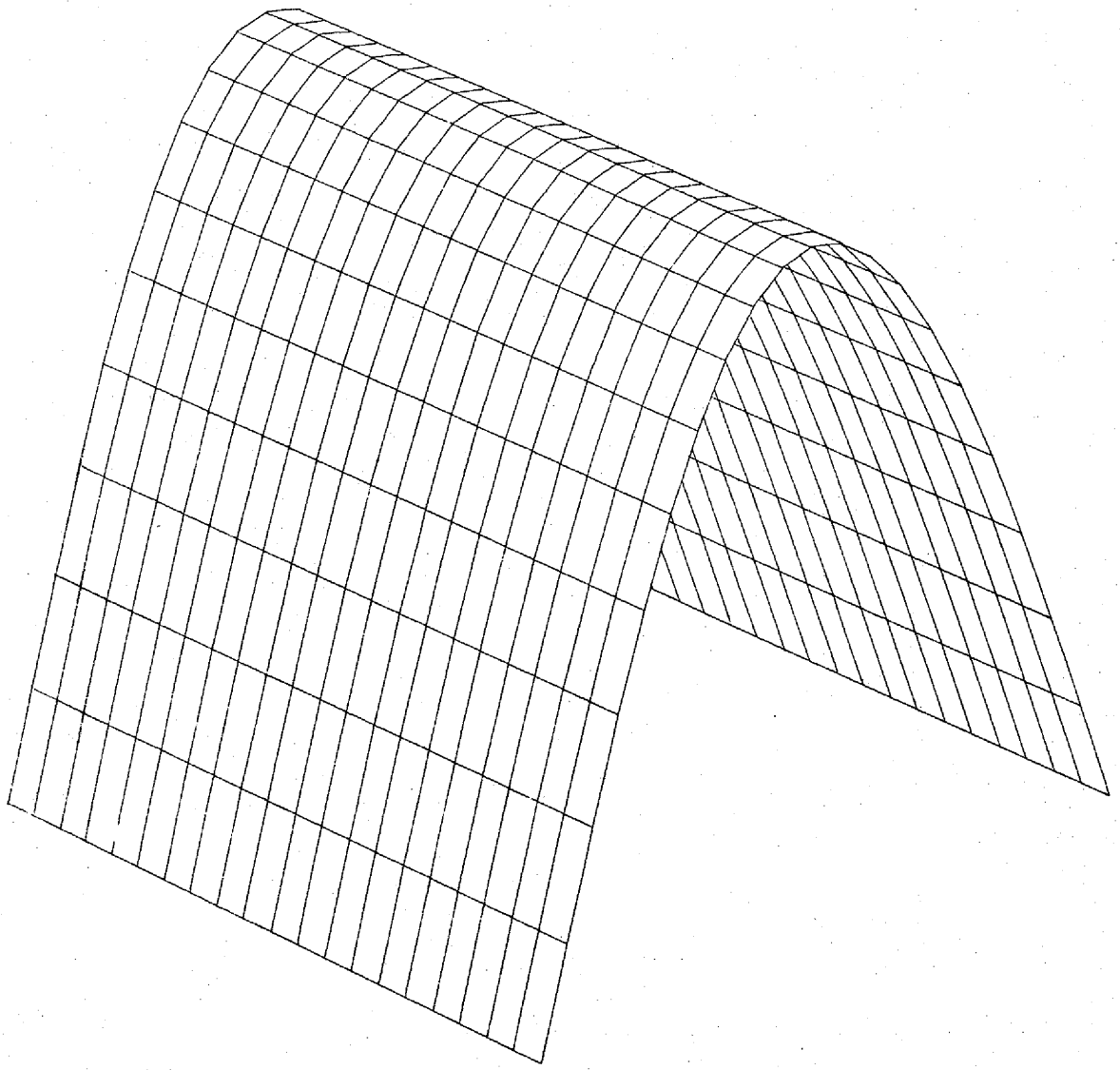

Figure 3. Initial data for the two-dimensional model problem.

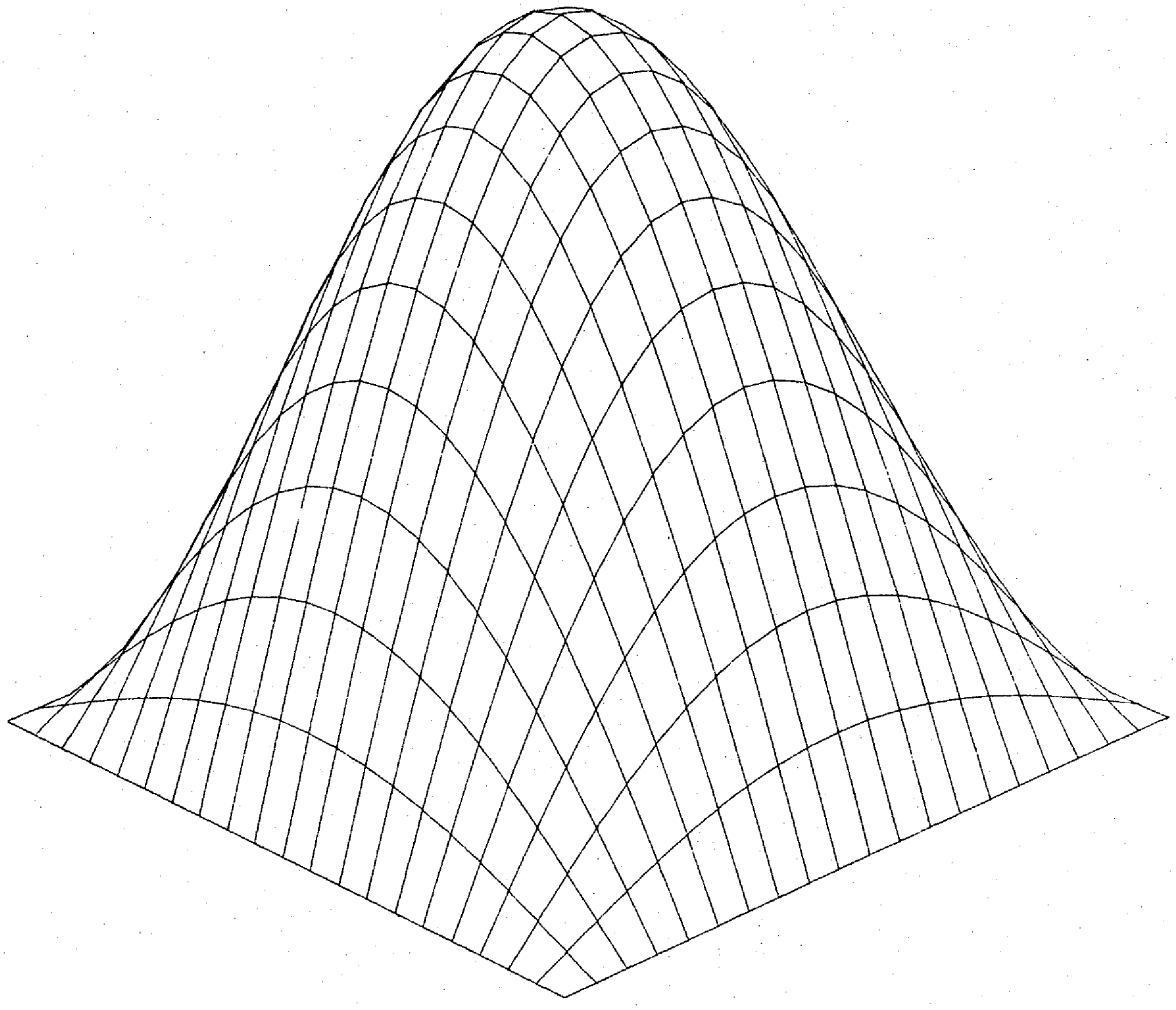

Figure 4. Theoretical solution to the model problem at $t = 1.0$.

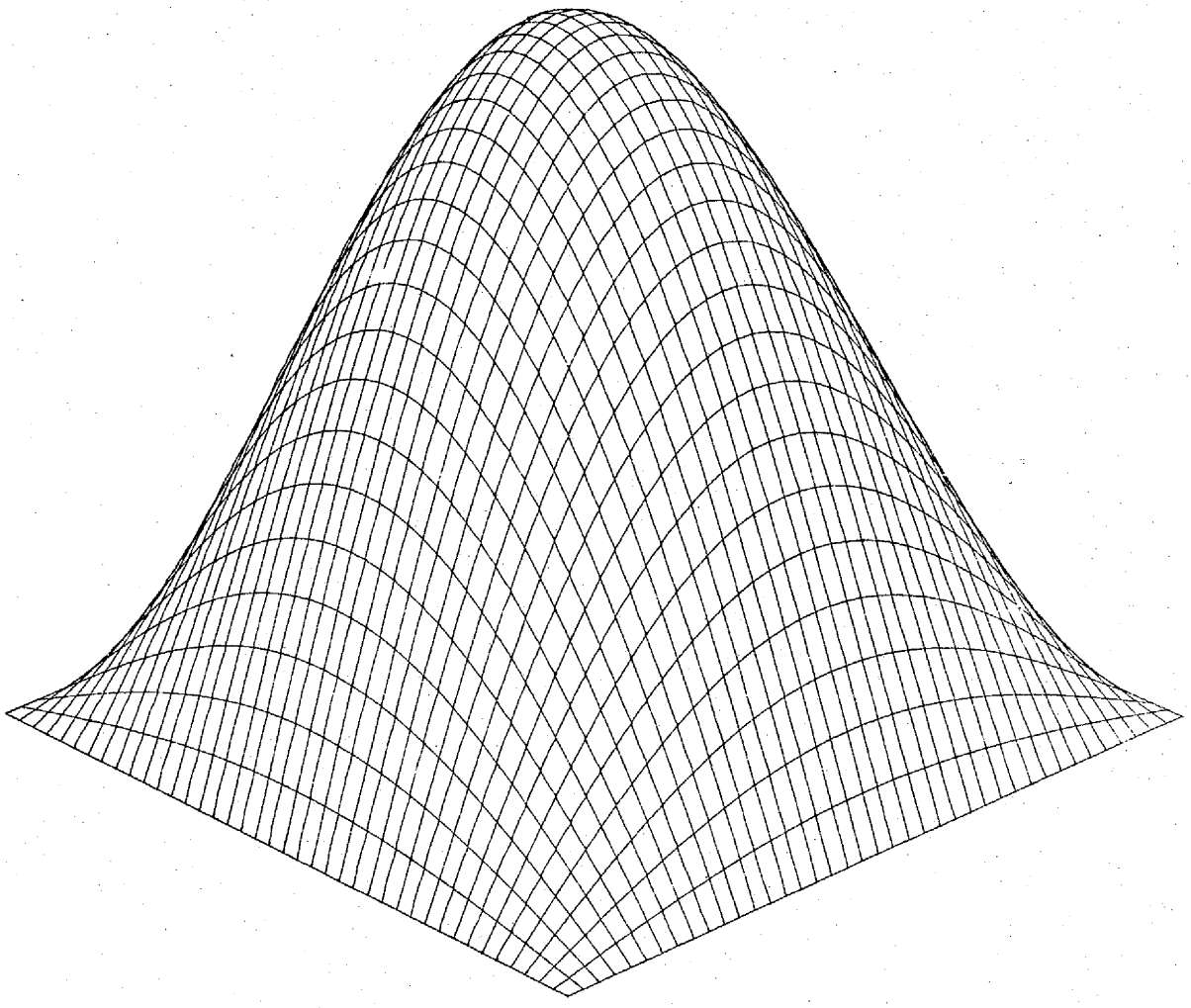

Figure 5. Backward-Difference solution with $h = 0.05$ and $\tau = 0.1$.

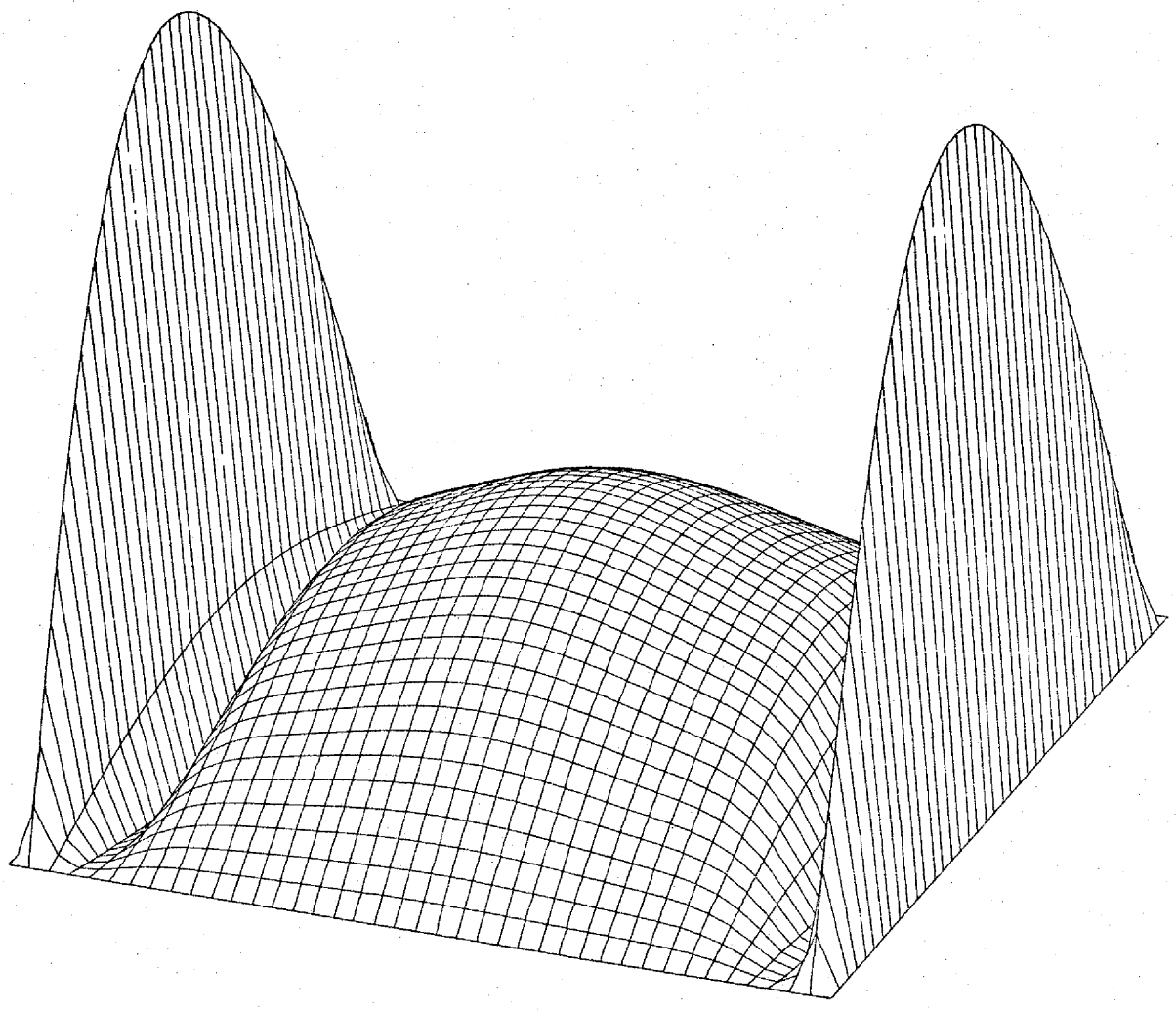

Figure 6. Peaceman-Rachford solution with $h = 0.05$ and $\tau = 0.1$.

It should be emphasized that the central portion of this figure is an accurate approximation to the theoretical solution so that rescaling has apparently decreased this portion of the solution in order to show the large peaks adjacent to the boundary on a graph of the same size. The numerical results obtained using the novel algorithm are depicted in figure 7 using $h = 0.05$. The general behaviour of the solution in this case is clearly very good. The maximum errors which occurred are summarized in table 2 where, it should be noted, the theoretical solution has a maximum value of approximately .01,

Method	$\tau = 0.1$			$\tau = 0.01$		
	h=0.1	h=0.05	h=0.025	h=0.1	h=0.05	h=0.025
Backward-Difference	.64E-02	.63E-02	.63E-02	.64E-03	.58E-03	.57E-03
Peaceman-Rachford	.47E-02	.23E-01	.46E-01	.72E-04	.16E-04	.55E-05
Novel Scheme	.94E-03	.88E-03	.87E-03	.91E-04	.35E-04	.22E-04

Table 2. Errors in solving the two-dimensional model problem at $t = 1$.

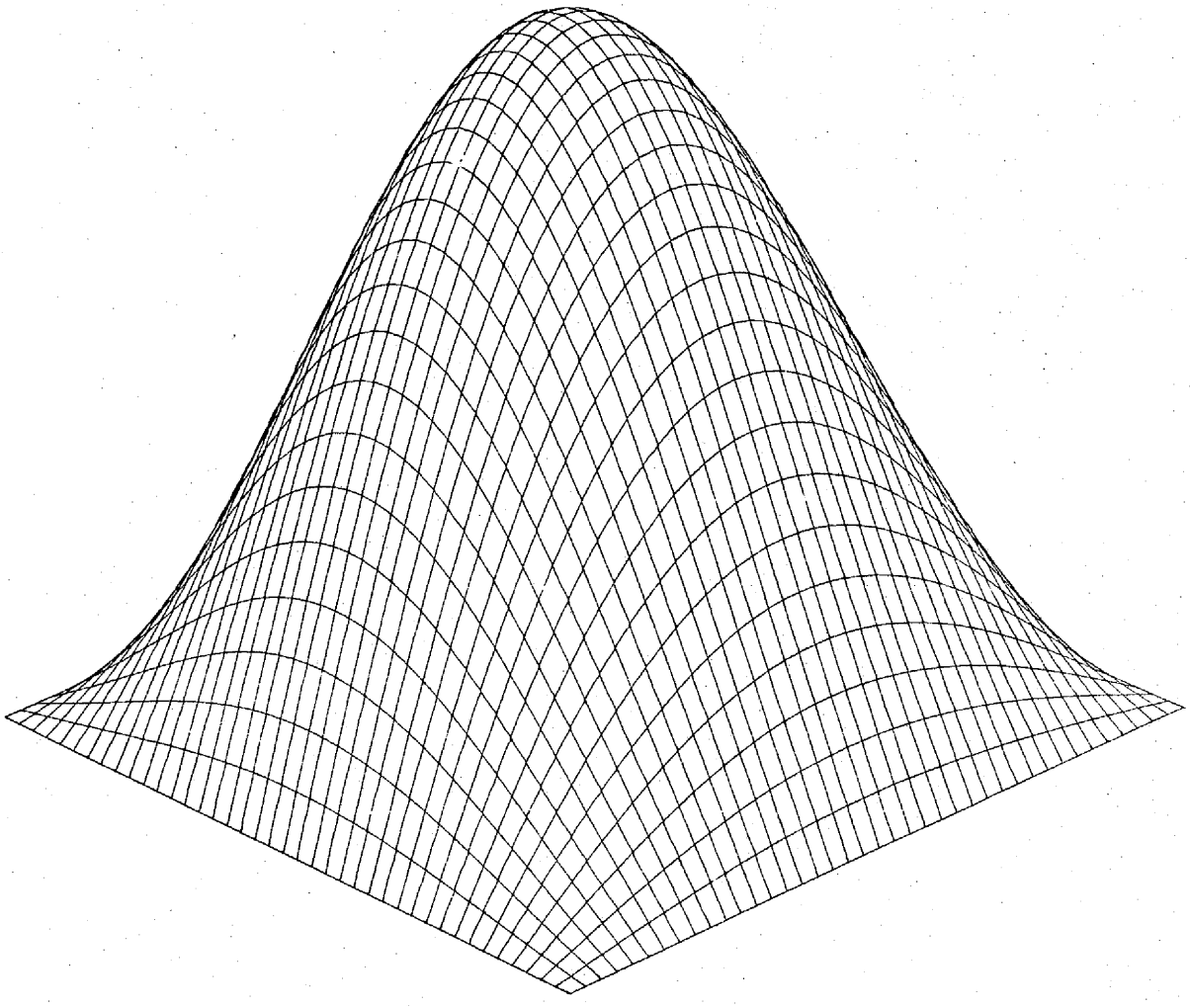

Figure 7. Extrapolation solution with $h = 0.05$ and $\tau = 0.1$.

4. Conclusions

We have derived a novel algorithm which is second order accurate in time as an extrapolation of a first order method, which is unconditionally stable and imposes no restriction on the time step as a function of the spatial discretization h. Our attention has been confined to the constant coefficient heat equation in one and two space variables. The generalization to higher space dimensions is straightforward. For example, if A is an $N^3 \times N^3$ matrix arising from a discretization of the three dimensional Laplacian and we write

$$A = A_1 + A_2 + A_3$$

then

$$v^{(0)} = \prod_{i=1}^{3} (I - \tau A_i)^{-1} \prod_{i=3}^{1} (I - \tau A_i)^{-1} \underset{\sim}{v}(t)$$

$$\underset{\sim}{v}^{(1)} = \prod_{i=1}^{3} (I - 2\tau A_i)^{-1} \underset{\sim}{v}(t)$$

$$v^{(2)} = \prod_{i=3}^{1} (I - 2\tau A_i)^{-1} \underset{\sim}{v}(t)$$

and $$\underset{\sim}{v}(t + 2\tau) = 2\underset{\sim}{v}^{(0)} - \frac{1}{2}(\underset{\sim}{v}^{(1)} + \underset{\sim}{v}^{(2)})$$

is second order accurate in time.

In a subsequent paper we will report on the generalizations to problems with inhomogeneous time-dependent boundary conditions and problems with inhomogeneous time-dependent source terms.

Acknowledgements

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