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NEW NUMERICAL METHOD FOR PARTIAL DIFFERENTIAL EQUATIONS. 1: APPLICATION TO THE DIFFUSION EQUATION

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SUMMARY

In this paper a new, highly accurate method called PH is presented for the numerical integration of partial differential equations. The method is applied for the solution of the one-dimensional diffusion equation. Upon integrating the equation within a subdomain of space and time using the prismoidal approximation, a three-point implicit scheme is obtained with a truncation error of order $O(k^4, h^6)$, where k and h represent the time and space steps respectively. The method is stable under the condition $s = \alpha k/h^2 \leqslant S(\delta)$, where the function $S(\delta)$ increases as the parameter δ decreases from $\frac{1}{12}$ to negative values. In practice the method behaves as unconditionally stable upon choosing an appropriate value for δ. A new formula is also adopted for the implementation of a Neumann boundary condition, introducing a truncation error of order $O(h^4)$. Numerical solutions are obtained incorporating Dirichlet and Neumann boundary conditions. The results prove that our method is far more accurate than any other implicit or explicit method.

INTRODUCTION

The significance of the application of numerical schemes of high accuracy for the computational solution of problems governed by partial differential equations is well known. Thus a large number of numerical methods have been derived within the finite difference and finite element frameworks, particularly for the solution of problems in fluid mechanics and heat transfer.

In constructing a numerical method, one encounters the question of stability and accuracy of the obtained numerical solutions. If a very restrictive stability condition has to be satisfied, the convergence of the numerical solution to the exact solution of a partial differential equation requires an enormous number of iterations for the complete integration of the problem. This has led to the development of various numerical schemes and their classification as methods of explicit and implicit type. The advantage of implicit schemes is that they are usually unconditionally stable, permitting the selection of an appropriate mesh which requires a reasonable number of iterations for the complete integration of the problem. To illustrate the basic characteristics of explicit and implicit schemes, we consider the one-dimensional diffusion equation, which incorporates the same dissipative behaviour as that of flow problems with significant viscous or heat conduction effects. The application of various numerical methods to the diffusion equation, the determination of the corresponding stability criterion and the estimation of the

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order of the truncation error provide guidance in choosing the appropriate numerical algorithm for the various viscous and heat transfer flow problems.

Let us consider the one-dimensional diffusion equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \tag{1}$$

where $u(x, t)$ may represent a quantity such as momentum, vorticity, mass or heat. If $u(x, t)$ represents the temperature as heat flows along an isolated rod of length $l = 1$, the constant α is the thermal diffusivity and x and t are the space and time variables respectively. The function $u(x, t)$ may be subjected to initial and Dirichlet boundary conditions of the form

$$u(x, t_0) = f(x), \qquad u(0, t) = C_0(t), \qquad u(1, t) = C_1(t), \tag{2}$$

where $f(x)$, $C_0(t)$ and $C_1(t)$ are known functions or constants. In the case where heat transfer is taking place from the end of the rod at $x = 0$, we can impose a Neumann boundary condition of the form

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

where $g(t)$ may be a constant. The accuracy of the implementation of the boundary condition (3) drastically affects the accuracy of the obtained solution.

Several explicit and implicit methods are extensively discussed in the books by Richtmyer and Morton,[1] Fletcher,[2] Ames[3] and Patankar.[4] The most popular explicit methods, listed in Table 7.1 of Reference 2 and in Table 8.1 of Reference 1, are the forward time-centred space (FTCS) and three-level (3L) schemes, which are conditionally stable for $s = \alpha k/h^2 \leqslant 1$ with a truncation error of order $O(k^2, h^2)$. Here k and h are the time and space steps respectively. The error can be reduced further to $O(k^2, h^4)$ using the more restrictive conditions $s = \frac{1}{6}$ and $s \leqslant 0{\cdot}35$ respectively. The more accurate 3L fourth-order (3L-4TH) scheme is described by equation (4) below after substitution of the term $L_{xx}u_i^{n+1}$ by $L_{xx}u_i^{n-1}$ and putting $\beta = -0{\cdot}5 - \gamma + 1/12s$. On the other hand, the fully implicit scheme, the Crank–Nicolson scheme and the generalized three-level (3LFI) scheme are unconditionally stable with truncation errors which vary from $O(k^2, h^2)$ to $O(k^2, h^4)$.

Other higher-order schemes have been constructed within the Galerkin finite element method using linear approximating functions. Following Fletcher,[2] we incorporate various finite difference and finite element three-level schemes in the equation

$$(1 + \gamma)M_x \frac{\Delta u_i^{n+1}}{k} - \gamma M_x \frac{\Delta u_i^n}{k} = \alpha[\beta L_{xx}u_i^{n+1} + (1 - \beta)L_{xx}u_i^n], \tag{4}$$

where $\Delta u_i^{n+1} = u_i^{n+1} - u_i^n$ and $L_{xx}u_i^n = (u_{i+1}^n - 2u_i^n + u_{i-1}^n)/h^2$. The mass operator M_x is defined as $M_x = \{\delta, 1 - 2\delta, \delta\}$, so that

$$M_x \Delta u_i^n = \delta \Delta u_{i+1}^n + (1 - 2\delta)\Delta u_i^n + \delta \Delta u_{i-1}^n. \tag{5}$$

Various schemes are obtained for different values of the parameters δ, β and γ. However, the most accurate unconditionally stable schemes, having fourth-order accuracy $O(k^2, h^4)$, are those listed in Table I with $\gamma = 0$ or 1.

In this paper we develop a new numerical implicit method which we call PH. This method is stable for $s \leqslant S(\delta)$, where the function $S(\delta)$ increases continuously to infinity as the parameter

Table I. Numerical schemes which are described by equation (4) and their corresponding parameters with $\gamma = 0$ or 1

Method	M_x	$\beta(\gamma)$
FDM-4TH	(0, 1, 0)	$\beta_{-}(\gamma) = 0{\cdot}5 + \gamma - 1/12s$
FEM-4TH	$(\frac{1}{6}, \frac{4}{6}, \frac{1}{6})$	$\beta_{+}(\gamma) = 0{\cdot}5 + \gamma + 1/12s$
COMP	$(\frac{1}{12}, \frac{10}{12}, \frac{1}{12})$	$0{\cdot}5 + \gamma$

δ decreases from $\frac{1}{12}$ to negative values. Thus we have a stability region with a varying upper limit. On the other hand, the method is highly accurate, having a truncation error of order $O(k^4, h^6)$. We also introduce a new approximation of higher accuracy for the implementation of boundary conditions of the Neumann type.

The extension of our method to the numerical treatment of problems with linear or non-linear convection and from one to three dimensions will be presented in a series of forthcoming papers.

DEVELOPMENT OF THE METHOD

Let us consider that the exact solution $u(x, t)$ of equation (1) is approximated by the finite difference solution $u_i^n = u(x_i, t_n)$, where $x_i = h(i-1)$ and $t_n = k(n-1)$ with $i = 1, 2, \ldots, I$ and $n = 1, 2, 3, \ldots, N$. Integrating equation (1) over x in the interval $x_{i-1} \leqslant x \leqslant x_{i+1}$ using the prismoidal formula

$$\int_{x_{i-1}}^{x_{i+1}} u\partial x = \frac{h}{3}(u_{i+1} + 4u_i + u_{i-1}) + O(h^5), \tag{6}$$

we have

$$\begin{aligned}\int_{x_{i-1}}^{x_{i+1}} \frac{\partial u}{\partial t}\,\mathrm{d}x &= \frac{h}{3}\left[\left(\frac{\partial u}{\partial t}\right)_{i+1} + 4\left(\frac{\partial u}{\partial t}\right)_i + \left(\frac{\partial u}{\partial t}\right)_{i-1}\right] = \alpha\int_{x_{i-1}}^{x_{i+1}} \frac{\partial^2 u}{\partial x^2}\,\mathrm{d}x = \alpha\left[\left(\frac{\partial u}{\partial x}\right)_{i+1} - \left(\frac{\partial u}{\partial x}\right)_{i-1}\right]\\ &= \alpha\left[2h\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{2h^3}{3!}\left(\frac{\partial^4 u}{\partial x^4}\right)_i + \frac{2h^5}{5!}\left(\frac{\partial^6 u}{\partial x^6}\right)_i + \cdots\right].\end{aligned} \tag{7}$$

Integrating equation (7) over t in the inerval $t_{n-1} \leqslant t \leqslant t_{n+1}$, we obtain

$$\frac{h}{3}(\Delta u_{i+1}^{n+1} + 4\Delta u_i^{n+1} + \Delta u_{i-1}^{n+1}) = 2h\alpha\int_{t_{n-1}}^{t_{n+1}}\left[\left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{h^2}{6}\left(\frac{\partial^4 u}{\partial x^4}\right)_i\right]\mathrm{d}t + O(h^5) = 2h\alpha I + O(h^5), \tag{8}$$

where $\Delta u_i^{n+1} = u_i^{n+1} - u_i^{n-1}$. Considering that

$$\frac{1}{h^2}L_{xx}u_i = \frac{1}{h^2}(u_{i+1} - 2u_i + u_{i-1}) = \left(\frac{\partial^2 u}{\partial x^2}\right)_i + \frac{2h^2}{4!}\left(\frac{\partial^4 u}{\partial x^4}\right)_i + O(h^4) \tag{9}$$

and $\partial^4 u/\partial x^4 = \alpha^{-2}\partial^2 u/\partial t^2$, because of (1), the integral I takes the form

$$I = \int_{t_{n-1}}^{t_{n+1}} \left(\frac{1}{h^2} L_{xx} u_i + \frac{h^2}{12\alpha^2} \frac{\partial^2 u}{\partial t^2}\right) dt = \frac{k}{3h^2} L_{xx}(u_i^{n+1} + 4u_i^n + u_i^{n-1}) + \frac{h^2}{12\alpha^2} \left[\left(\frac{\partial u}{\partial t}\right)_i^{n+1} - \left(\frac{\partial u}{\partial t}\right)_i^{n-1}\right]$$

$$= \frac{k}{3h^2} L_{xx}(u_i^{n+1} + 4u_i^n + u_i^{n-1}) + \frac{h^2}{6\alpha k} L_{tt} u_i^n, \tag{10}$$

where $L_{tt} u_i^n = u_i^{n+1} - 2u_i^n + u_i^{n-1}$. The last step of equation (10) was obtained by using the approximation

$$\left(\frac{\partial u}{\partial t}\right)_i^{n+1} - \left(\frac{\partial u}{\partial t}\right)_i^{n-1} = 2k\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n + \frac{2k^3}{6}\left(\frac{\partial^4 u}{\partial t^4}\right)_i^n + O(k^5) = \frac{2}{k} L_{tt} u_i^n + \frac{k^3}{12}\left(\frac{\partial^4 u}{\partial t^4}\right)_i + O(k^5) \tag{11}$$

and neglecting terms of order equal to or higher than $O(h^2, k^3)$. Substituting equation (10) into equation (8), we obtain the final three-level implicit scheme

$$\frac{1}{6k}(\Delta u_i^{n+1} + 4\Delta u_i^{n+1} + \Delta u_i^{n+1}) = \frac{\alpha}{3h^2} L_{xx}(u_i^{n+1} + 4u_i^n + u_i^{n-1}) + \frac{h^2}{6\alpha k^2} L_{tt} u_i^n. \tag{12}$$

In constructing this equation, we have neglected terms of order equal to or higher than $O(k^2, h^2)$ and $O(k^4, h^4)$. However, the von Neumann stability analysis below indicates that the scheme is unconditionally unstable for $s = \alpha k/h^2 > 0$. This is due to the specific numerical coefficients $\frac{1}{6}$, $\frac{1}{3}$ and $\frac{1}{6}$ which multiply the respective terms of equation (12).

Thus instead of equation (12) we adopt the modified equation

$$\frac{\delta}{k}[\Delta u_{i+1}^{n+1} + (1 - 2\delta)\Delta u_i^{n+1} + \delta \Delta u_{i-1}^{n+1}] = \frac{2\alpha}{h^2}[\beta L_{xx} u_i^{n+1} + (1 - 2\beta) L_{xx} u_i^n + \beta L_{xx} u_i^{n-1}]$$

$$+ \frac{\eta h^2}{\alpha k^2} L_{tt} u_i^n, \tag{13}$$

where the interelations between the parameters δ, β and η are going to be determined later.

Defining the mass operators as

$$M_x \equiv \{\delta, 1 - 2\delta, \delta\}, \qquad M_t \equiv \{\beta, 1 - 2\beta, \beta\}, \tag{14}$$

so that

$$M_t L_{xx} u_i^n = \beta L_{xx} u_i^{n+1} + (1 - 2\beta) L_{xx} u_i^n + \beta L_{xx} u_i^{n-1} = L_{xx} M_t u_i^n, \tag{15}$$

equation (13) can be written in the compact form

$$M_x \Delta u_i^{n+1} = 2s L_{xx} M_t u_i^n + \frac{\eta}{s} L_{tt} u_i^n. \tag{16}$$

The advantage of equation (16) is that it is applied at every node, producing a tridiagonal system of equations of the form

$$c_1 u_{i-1}^{n+1} + c_2 u_i^{n+1} + c_1 u_{i+1}^{n+1} = c_3 u_{i-1}^n + c_4 u_i^n + c_3 u_{i+1}^n + c_5 u_{i-1}^{n-1} + c_6 u_i^{n-1} + c_5 u_{i+1}^{n-1}, \tag{17}$$

with

$$c_1 = \delta - 2\beta s, \qquad c_3 = 2s(1 - 2\beta), \qquad c_5 = \delta + 2\beta s,$$

$$c_2 = 1 - 2\delta + 4\beta s - \frac{\eta}{s}, \qquad c_4 = -4s(1 - 2\beta) - \frac{2\eta}{s}, \qquad c_6 = 1 - 2\delta - 4\beta s + \frac{\eta}{s},$$

which can be solved using the Thomas algorithm.

In studying below the accuracy of the method (16), we shall determine the functions $\beta = \beta(\delta)$ and $\eta = \eta(\delta)$ for which the truncation error is reduced to $O(k^4, h^6)$. The best values of the parameter δ will be determined from the required stability condition on s.

Following our integration method, by expressing the functions u_i^n in terms of u_i^{n+1} and u_i^{n-1} via Taylor series expansions and strictly neglecting terms of order equal to or higher than $O(k^2, h^4)$, we can produce the equation of the composite (COMP) scheme.

TRUNCTATION ERROR AND STABILITY CONDITION

We denote the diffusion equation (1) and its discretized form (13) by $D(u) = 0$ and $F(u) = 0$ respectively. Substituting $\bar{u}_i^n$, the exact solution of equation (1) at the node (i, n), into $F(\bar{u}_i^n) = 0$ and expressing all the terms in Taylor series expansions about the node (i, n), we produce the truncation error

$$E_i^n = F(\bar{u}_i^n) - D(\bar{u}_i^n). \tag{18}$$

Thus, expressing $\bar{u}_{i+1}^n$ and $\bar{u}_{i-1}^n$ in Taylor series with respect to $\bar{u}_i^n$, we have

$$\delta\bar{u}_{i+1}^n + (1 - 2\delta)\bar{u}_i^n + \delta\bar{u}_{i-1}^n = \bar{u}_i^n + \delta h^2\left(\frac{\partial^2\bar{u}}{\partial x^2}\right)_i^n + \frac{\delta h^4}{12}\left(\frac{\partial^4\bar{u}}{\partial x^4}\right)_i^n + \frac{2\delta h^6}{6!}\left(\frac{\partial^6\bar{u}}{\partial x^6}\right)_{i+\theta}^n, \tag{19}$$

where the last term is the remainder of the series with $0 < \theta < 1$. Applying equation (19) in the case of $\Delta u^{n+1}/k$, we have

$$\frac{1}{k}[\delta\Delta\bar{u}_{i+1}^{n+1} + (1 - 2\delta)\Delta\bar{u}_i^{n+1} + \delta\Delta\bar{u}_{i-1}^{n+1}] = \left(\frac{\Delta\bar{u}}{k}\right)_i^{n+1} + \delta h^2\frac{\partial^2}{\partial x^2}\left(\frac{\Delta\bar{u}}{k}\right)_i^{n+1} + \frac{\delta h^4}{12}\frac{\partial^4}{\partial x^4}\left(\frac{\Delta\bar{u}}{k}\right)_i^{n+1} + O(h^6). \tag{20}$$

Similarly, expressing $\bar{u}_i^{n+1}$ and $\bar{u}_i^{n-1}$ in Taylor series with respect to $\bar{u}_i^n$, we obtain the relation

$$\frac{1}{h^2}[\beta L_{xx}\bar{u}_i^{n+1} + (1 - 2\beta)L_{xx}\bar{u}_i^n + \beta L_{xx}\bar{u}_i^{n-1}] = \left(\frac{L_{xx}\bar{u}}{h^2}\right)_i^n + \beta k^2\frac{\partial^2}{\partial t^2}\left(\frac{L_{xx}\bar{u}}{h^2}\right)_i^n + \beta k^4\frac{\partial^4}{\partial t^4}\left(\frac{L_{xx}\bar{u}}{h^2}\right)_i^n + O(k^6). \tag{21}$$

The quantities $\Delta\bar{u}_i^{n+1}$, $L_{xx}\bar{u}_i^n$ and $L_{tt}\bar{u}_i^n$ in equations (20), (21) and (16) are expressed in terms of the partial derivatives of $\bar{u}_i^n$ using the Taylor approximations

$$\frac{1}{k}\,\Delta\bar{u}_i^{n+1} = 2\left(\frac{\partial \bar{u}}{\partial t}\right)_i^n + \frac{k^2}{3}\left(\frac{\partial^3 \bar{u}}{\partial t^3}\right)_i^n + \frac{2k^4}{5!}\left(\frac{\partial^5 \bar{u}}{\partial t^5}\right)_i^n + O(k^5), \tag{22}$$

$$\frac{1}{h^2}\,L_{xx}\bar{u}_i^n = \left(\frac{\partial^2 \bar{u}}{\partial x^2}\right)_i^n + \frac{h^2}{12}\left(\frac{\partial^4 \bar{u}}{\partial x^4}\right)_i^n + \frac{2h^4}{6!}\left(\frac{\partial^6 \bar{u}}{\partial x^6}\right)_i^n + O(h^5), \tag{23}$$

$$\frac{1}{k^2}\,L_{tt}\bar{u}_i^n = \left(\frac{\partial^2 \bar{u}}{\partial t^2}\right)_i^n + \frac{k^2}{12}\left(\frac{\partial^4 \bar{u}}{\partial t^4}\right)_i^n + \frac{2k^4}{6!}\left(\frac{\partial^6 \bar{u}}{\partial t^6}\right)_i^n + O(k^5). \tag{24}$$

Substituting these quantities successively into equations (20), (21) and (13) and neglecting terms of order $O(k^m, h^v)$ with $m + v \geqslant 6$, we obtain the final expression for the truncation error (18) as

$$E_i^n = \alpha h^2\left(2\delta - \frac{1}{6} - \eta\right)\frac{\partial^4 \bar{u}}{\partial x^4} + \alpha^3 k^2\left[\frac{1}{3} - 2\beta + \frac{1}{6s^2}\left(\delta - \frac{1}{30}\right)\right]\frac{\partial^6 \bar{u}}{\partial x^6} + \frac{\alpha s^2 h^6}{6}\left(2\delta - \beta - \frac{\eta}{2}\right)\frac{\partial^8 \bar{u}}{\partial x^8}$$
$$+ \alpha^5 k^4\left[\frac{1}{60} - \frac{\beta}{6} + \frac{1}{36s^2}\left(\delta - \frac{\beta}{10\alpha}\right)\right]\frac{\partial^{10} \bar{u}}{\partial x^{10}}. \tag{25}$$

If the first two terms of (25) become equal to zero for

$$\eta = 2\delta - \tfrac{1}{6}, \qquad \beta = \frac{1}{6} + \frac{1}{12s^2}\left(\delta - \frac{1}{30}\right), \tag{26}$$

the truncation error of our scheme is reduced to $O(k^4, h^6)$. If in addition to equation (25) we put $2\delta - \beta - \eta/2 = 0$, we obtain the relation $\delta = (30s^2 - 1)/30(12s^2 - 1)$. In this case the truncation error is reduced further to $O(k^4, h^8)$ and the method is subjected to the stability condition $s \leqslant 1/\sqrt{12}$, which imposes a severe restriction on the choice of k for a given h.

The stability of the method is studied by applying a von Neumann analysis to the interior points. Thus the error $\xi_i^n = u_i^n - (u_i^n)^*$ between the solution u_i^n of equation (13) and that which is actually calculated, $(u_i^n)^*$, is expressed as a finite Fourier series

$$\xi_i^n = \sum_{m=1}^{I-2} e^{\lambda nk} e^{\sqrt{(-1)}\theta_m i}, \qquad \theta_m = m\pi h, \tag{27}$$

along the grid line $i = 2, 3, \ldots, I - 1$ at the nth time level. Since equation (1) is linear, a single Fourier component is introduced in the sum (27), i.e. $\xi_i^n = (G)^n e^{\sqrt{(-1)}\theta i}$, where $G = e^{\lambda k}$. It is noted that $\xi^{n+1}/\xi^n = G$ and $(G)^n$ represents G to the power n. The round-off errors associated with this scheme are propagated with equation (13).

Hence, substituting ξ_i^n into equation (13), dividing the resulting equation by $G^n e^{\sqrt{(-1)}\theta i}$ and putting $x = \cos\theta$, we obtain after some algebraic manipulations the equation

$$aG^2 + bG + c = 0 \quad \text{with } G = (-b \pm \sqrt{\Delta})/2a, \tag{28}$$

where

$$a = \frac{1}{3s}[2(1-x)s^2 + \gamma s + \varepsilon], \qquad b = \frac{1}{3s}[8(1-x)s^2 - 2\varepsilon], \qquad c = \frac{1}{3s}[2(1-x)s^2 - \gamma s + \varepsilon],$$

$$\gamma = 3 - 6\delta(1-x), \qquad \varepsilon = -6(\delta - \tfrac{1}{12}) + (\delta - \tfrac{1}{30})(1-x), \tag{29}$$

$$\Delta = \tfrac{4}{3}[12(1-x)^2 s^2 - 12(1-x)\varepsilon + \gamma^2].$$

For $\delta \leqslant \frac{1}{12}$ we have $\varepsilon \geqslant 0$, $\gamma > 0$ and $a \geqslant 0$ for every x in the region $-1 \leqslant x \leqslant 1$.

The stability requirement is $|G| \leqslant 1$ for all x. A detailed investigation indicates that if $a \geqslant 0$ and $\Delta \geqslant 0$, the coefficient b varies from positive to negative values as x increases from -1 to $+1$. However, for $b < 0$ the inequalities $-b + \sqrt{\Delta} \leqslant 0$ and $-b - \sqrt{\Delta} \geqslant 0$ do not hold when $ac < 0$. Thus G is given by equation (28) with $-b + \sqrt{\Delta} \geqslant 0$ or $-b - \sqrt{\Delta} \leqslant 0$ and stability of the solution is achieved under the conditions

$$0 \leqslant G \leqslant 1 \quad \text{for } 2a \geqslant -b \text{ and } a + b + c \geqslant 0, \tag{30}$$

$$-1 \leqslant G \leqslant 0 \quad \text{for } 2a \geqslant b \text{ and } a + c \geqslant b. \tag{31}$$

For $0 \leqslant G \leqslant 1$ the conditions (30) always hold because $2a + b = 6(1 - x)s^2 + \gamma s \geqslant 0$ and $a + b + c = 4s(1 - x) \geqslant 0$. For $-1 \leqslant G \leqslant 0$ the required conditions are satisfied if

$$a + c - b = \frac{4}{3s}\,[-(1 - x)s^2 + \varepsilon] \geqslant 0 \quad \text{or} \quad s^2 \leqslant \frac{\varepsilon}{1 - x} \quad \text{with } 1 - x \neq 0. \tag{32}$$

For $x = 1$ we have $\varepsilon \geqslant 0$, which is true for $\delta \leqslant \frac{1}{12}$. From (32) we have that $(1 - x)s^2 \leqslant \varepsilon \leqslant \varepsilon + \gamma s/2$, which shows that the condition $2a - b = -4(1 - x)s^2 + 2\gamma s + 4\varepsilon \geqslant 0$ is satisfied. In the case $\Delta < 0$ the condition $|G| = |GG^*| = (c/a)^{1/2} \leqslant 1$ is always satisfied when $a \geqslant 0$. When $-1 \leqslant G \leqslant 0$, the solution will have a decaying amplitude of oscillating sign as $n \to \infty$.

The inequality (32) represents the stability condition of our scheme and is written as

$$s \leqslant \left[\delta\left(\frac{-5 - x}{1 - x}\right) + \frac{14 + x}{30(1 - x)}\right]^{1/2}. \tag{33}$$

Considering that the right-hand side of (33) becomes minimum for $x = -1$, the stability condition takes the form

$$s \leqslant S(\delta) = -2\delta + \tfrac{13}{60} \quad \text{with } \delta \leqslant \tfrac{1}{12}. \tag{34}$$

Consequently the function $S(\delta)$ determines the upper limit of the stability region for s. It is clear that the stability region increases as δ decreases from $\frac{1}{12}$ to negative values. The variations in the functions $\eta(\delta)$, $\beta(\delta)$ and $S(\delta)$ for some of the most interesting values of δ are given in Table II. In practice our method behaves as an unconditionally stable implicit scheme upon choosing an appropriate value for δ.

Table II. Parametric values of $\eta(\delta)$, $\beta(\delta)$ and of $S(\delta)$, which is the upper limit of the stability region in our method

δ	η	$\beta(s = \frac{1}{6})$	$\beta(s = 1)$	$S(\delta)$
$\frac{1}{30}$	−0·100	0·166	0·166	0·387298
$-\frac{1}{30}$	−0·233	−0·033	0·161	0·532290
$-\frac{1}{6}$	−0·500	−0·433	0·150	0·741619
$-\frac{1}{2}$	−1·166	−1·433	0·122	1·103026
−1	−2·166	−2·933	0·080	1·488847

NEW NEUMANN BOUNDARY CONDITION APPROXIMATION

Before proceeding to the computational application of our scheme, we note that algorithm (13) is applied to internal nodes. At the boundary nodes the application of Dirichlet boundary conditions of the form (2) does not create any difficulty, because the only values required are $u_i^n = C_0^n$ and $u_l^u = C_1^n$ at nodes 1 and l respectively. However, in the case of Neumann boundary conditions of the form (3) a knowledge of the solution outside the computational domain is required. In the case of a Neumann boundary condition $\partial u(0, t)/\partial x = g(t)$ at the node $(i = 1, n)$, one of the following two formulae is used:

$$\frac{u_2^n - u_1^n}{h} = g^n \quad \text{or} \quad u_1^n = u_2^n - hg^n, \tag{35}$$

$$\frac{u_2^n - u_0^n}{2h} = g^n \quad \text{or} \quad u_0^n = u_2^n - 2hg^n, \tag{36}$$

introducing a truncation error of order $O(h)$ and $O(h^2)$ respectively. In both cases equation (35) or (36) is combined with a numerical scheme centred at the node $(1, n)$ for the elimination of terms such as u_1^n or u_0^n. However, the use of (35) or (36) in conjuction with a numerical algorithm of higher accuracy results in the propagation of the corresponding error along the x-grid line for all later times, thus dramatically reducing the accuracy of the method.

To avoid the previous disadvantageous, we present a new technique for the implementation of a Neumann boundary condition. Integrating equation (3) using the formula (6), we have

$$\begin{aligned}\int_{x_{i-1}}^{x_{i+1}} \frac{\partial u}{\partial x}\,\mathrm{d}x = \int_{x_{i-1}}^{x_{i+1}} \mathrm{d}u = u_{i+1} - u_{i-1} &= \frac{h}{3}\left[\left(\frac{\partial u}{\partial x}\right)_{i+1} + 4\left(\frac{\partial u}{\partial x}\right)_i + \left(\frac{\partial u}{\partial x}\right)_{i-1}\right] \\ &= \frac{h}{3}\left[6\left(\frac{\partial u}{\partial x}\right)_i + h^2\left(\frac{\partial^3 u}{\partial x^3}\right)_i + O(h^4)\right] + O(h^5).\end{aligned} \tag{37}$$

Substitution of $\partial^2 u/\partial x \partial t = \alpha \partial^3 u/\partial x^3$ into equation (37) yields the final formula

$$u_{i+1}^n - u_{i-1}^n = \frac{h}{3}\left[6\left(\frac{\partial u}{\partial x}\right)_i^n + \frac{h^2}{\alpha}\frac{\partial}{\partial t}\left(\frac{\partial u}{\partial x}\right)_i^n\right] \tag{38}$$

with a truncation error of $O(h^5)$. The term $(\partial u/\partial x)_i^n$ is the known boundary condition at the node i. If we assume that there are Neumann boundary conditions at the end points of the interval $x_1 \leq x \leq x_l$ given by

$$\frac{\partial u(x_1, t)}{\partial x} = g_1(t), \qquad \frac{\partial u(x_l, t)}{\partial x} = g_2(t), \tag{39}$$

their corresponding approximate formulae at x_1 and x_l are written via (38) as

$$u_2^n - u_0^n = \frac{h}{3}\left[6g_1^n + \frac{h^2}{\alpha}\left(\frac{\partial g_1}{\partial t}\right)^n\right], \tag{40a}$$

$$u_{l+1}^n - u_{l-1}^n = \frac{h}{3}\left[6g_2^n + \frac{h^2}{\alpha}\left(\frac{\partial g_2}{\partial t}\right)^n\right]. \tag{40b}$$

Using these relations, the values of u_0^n and u_{l+1}^n are eliminated from the algebraic equations of the interior points.

The method which we have developed above can be generalized to the case of more complicated partial differential equations than the diffusion equation.

RESULTS AND DISCUSSION

Numerical results have been obtained with our PH scheme using Dirichlet and Neumann boundary conditions. These results are compared with those obtained with the aforementioned (see Introduction) explicit and implicit schemes as well as with the corresponding exact solutions.

We begin our study by considering the transient heat conduction along an insulated rod which is in contact at its two ends with two hot reservoirs. The temperature $u(x, t)$ governed by equation (1) is subject to Dirichlet boundary conditions

$$u(0, t) = u(1, t) = 100\ ^{\circ}\mathrm{C}, \tag{41}$$

with initial temperature $u(x, 0) = 0\ ^{\circ}\mathrm{C}$ and thermal diffusivity $\alpha = 0{\cdot}01$. The exact solution of the problem is given by[2]

$$u_{\mathrm{ex}}(x_i, t_n) = 100 - \sum_{m=1}^{10} \frac{400}{(2m-1)\pi} \sin[(2m-1)\pi x_i] e^{-\alpha(2m-1)^2\pi^2 t_n^2}. \tag{42}$$

The RMS error between the exact and the numerical solution is evaluated from the formula

$$\mathrm{RMS} = \left(\sum_{i=1}^{I} (u_i - u_{\mathrm{ex}_i})^2 / I \right)^{1/2} \tag{43}$$

Applying our method to u_i^n with $n \geq 3$, we calculate u_i^1 from the initial conditions and u_i^2 from the application of the COMP method. The variations in $u(x, t)$ along the rod at $t = 4{\cdot}5$ and $12{\cdot}5$ are shown in Figure 1. The accuracy of our PH scheme (13) is estimated by studying the calculated RMS errors (Table III) at $t = 12$ for grids with $h = 0{\cdot}05$, $0{\cdot}1$ and $0{\cdot}2$ and parametric values $s = 0{\cdot}166$, $0{\cdot}3$, $0{\cdot}5$, 1 and $\delta = \frac{1}{30}, -\frac{1}{30}, -\frac{1}{6}, -\frac{1}{2}, -1$. These results were obtained with the initial condition defined by the exact solution (42) at $t = 4{\cdot}5$ in order to avoid errors in

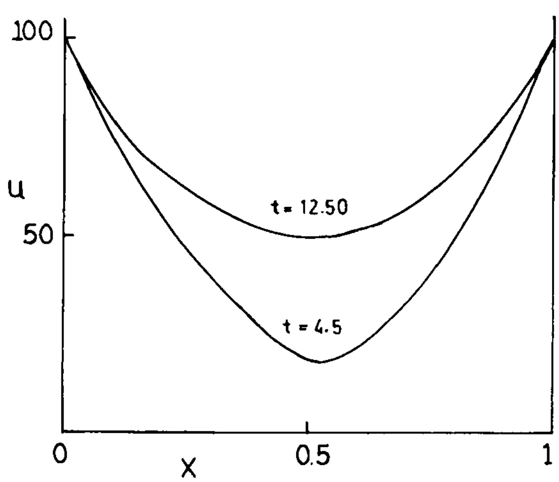

Figure 1. Variation in $u(x, t)$ subject to Dirichlet boundary conditions $u(0, t) = u(1, t) = 100\ ^{\circ}\mathrm{C}$ at $t = 4{\cdot}5$ and $12{\cdot}5$

Table III. Estimation of the accuracy of our method subject to the Dirichlet boundary conditions (41) at $t = 12$

S	δ	RMS ($\theta = 0{\cdot}2$)	RMS ($h = 0{\cdot}1$)	RMS ($h = 0{\cdot}05$)	r
$\frac{1}{6}$	$\frac{1}{30}$	0·000480	$0{\cdot}763904 \times 10^{-5}$	$0{\cdot}127209 \times 10^{-6}$	5.9
	$-\frac{1}{30}$	0·000557	$0{\cdot}853179 \times 10^{-5}$	$0{\cdot}140273 \times 10^{-6}$	5.9
	$-\frac{1}{6}$	0·000780	$0{\cdot}105388 \times 10^{-4}$	$0{\cdot}167693 \times 10^{-6}$	5.9
	$-\frac{1}{2}$	0·001576	$0{\cdot}170252 \times 10^{-4}$	$0{\cdot}242563 \times 10^{-6}$	6.1
	-1	0·002518	$0{\cdot}317568 \times 10^{-4}$	$0{\cdot}369892 \times 10^{-6}$	6.4
0·3	$\frac{1}{30}$	0·000815	$0{\cdot}105364 \times 10^{-4}$	$0{\cdot}165030 \times 10^{-6}$	5.9
	$-\frac{1}{30}$	0·000822	$0{\cdot}122489 \times 10^{-4}$	$0{\cdot}190026 \times 10^{-6}$	6·0
	$-\frac{1}{6}$	0·001277	$0{\cdot}160599 \times 10^{-4}$	$0{\cdot}241909 \times 10^{-6}$	6·0
	$-\frac{1}{2}$	0·002783	$0{\cdot}281840 \times 10^{-4}$	$0{\cdot}381190 \times 10^{-6}$	6·2
	-1	0·004433	$0{\cdot}551824 \times 10^{-4}$	$0{\cdot}614881 \times 10^{-6}$	6·4
0·5	$\frac{1}{30}$	0·040334	0·000108	0·000168	−0·6
	$-\frac{1}{30}$	0·013143	0·000114	$0{\cdot}182929 \times 10^{-5}$	5·9
	$-\frac{1}{6}$	0·008127	0·000133	$0{\cdot}208336 \times 10^{-5}$	6·0
	$-\frac{1}{2}$	0·014768	0·000193	$0{\cdot}276851 \times 10^{-5}$	6·1
	-1	0·23259	0·000325	$0{\cdot}392451 \times 10^{-5}$	6·3
1·0	$\frac{1}{30}$	0·210527	0·016112	0·254131	−3·9
	$-\frac{1}{30}$	0·183352	0·002857	0·001852	0·6
	$-\frac{1}{6}$	0·154849	0·001036	0·000018	5·8
	$-\frac{1}{2}$	0·146756	0·001271	0·000021	5·9
	-1	0·164526	0·001791	0·000026	6·0

implementing the boundary conditions and for comparison with other similar results in Table V. The approximate convergence rate expressing the ratio of the RMS errors for $h = 0{\cdot}1$ and 0·05 is given by[2]

$$r = \ln(\mathrm{RMS}_{h=0\cdot1}/\mathrm{RMS}_{h=0\cdot05})/\ln 2 \tag{44}$$

and is also presented in Table V. We observe that the accuracy of the scheme is increased even for large values of h as s decreases. For a specific value of s the accuracy of the method increases upon choosing a value for δ for which the upper limit of the stability region $S(\delta)$ is nearer to s. On the other hand, as s increases to values larger than $S(\delta)$ for a specific value of δ, instabilities are introduced in the numerical solution, yielding large RMS errors. This is more pronounced when $s = 1$ and $\delta = \frac{1}{30}$, for which $S(\delta) = 0{\cdot}387$, yielding a negative r. However, these instabilities are reduced smoothly as the step h increases. It is clear that for $s \leq 0{\cdot}3$ the error behaves like h^6.

In Table IV the error distributions $(u - u_{ex})_i^n$ are given at $t = 12{\cdot}5$ for grids with $h = 0{\cdot}1$ and 0·2 and parametric values $s = 0{\cdot}3$, 1 and $\delta = \frac{1}{30}, -\frac{1}{2}$. For $s = 1$ the error is larger at $\delta = \frac{1}{30}$ than that at $\delta = -\frac{1}{2}$ near the boundaries because of the strong induced instabilities at $\delta = \frac{1}{30}$. For $s = 0{\cdot}3$, which is well within the stability range determined by $\delta = \frac{1}{30}$ and $-\frac{1}{6}$, the error becomes larger at the middle of the rod.

The accuracy of our scheme is compared with that of the implicit schemes FDM-4TH, FEM-4TH and COMP and with the accuracy of the explicit schemes FTCS and 3L-4TH in Table V. All these methods have been described in the Introduction. The results of the methods with an asterisk have been taken from Reference 2, while the results of the PH and COMP

Table IV. Error distribution $(u - u_{ex})_i$ of our solution subject to the Dirichlet boundary conditions (41) at $t = 12{\cdot}5$

$x = 0$		0·2	0·4	0·6	0·8	1
$s = 1$, $\delta = \frac{1}{30}$	0	$-2{\cdot}238 \times 10^{-2}$	$1{\cdot}453 \times 10^{-2}$	$1{\cdot}453 \times 10^{-2}$	$-2{\cdot}238 \times 10^{-2}$	0
$h = 0{\cdot}1$, $\delta = -\frac{1}{2}$	0	$9{\cdot}511 \times 10^{-4}$	$1{\cdot}882 \times 10^{-3}$	$1{\cdot}882 \times 10^{-3}$	$9{\cdot}511 \times 10^{-4}$	0
$s = 1$, $\delta = \frac{1}{30}$	0	$-3{\cdot}456 \times 10^{-1}$	$1{\cdot}162 \times 10^{-1}$	$1{\cdot}162 \times 10^{-1}$	$-3{\cdot}456 \times 10^{-1}$	0
$h = 0{\cdot}2$, $\delta = -\frac{1}{2}$	0	$-7{\cdot}621 \times 10^{-2}$	$2{\cdot}425 \times 10^{-1}$	$2{\cdot}425 \times 10^{-1}$	$-7{\cdot}621 \times 10^{-2}$	0
$s = 0{\cdot}3$, $\delta = \frac{1}{30}$	0	$7{\cdot}542 \times 10^{-6}$	$1{\cdot}374 \times 10^{-5}$	$1{\cdot}373 \times 10^{-5}$	$7{\cdot}531 \times 10^{-6}$	0
$h = 0{\cdot}1$, $\delta = -\frac{1}{2}$	0	$1{\cdot}117 \times 10^{-5}$	$3{\cdot}620 \times 10^{-5}$	$3{\cdot}619 \times 10^{-5}$	$1{\cdot}116 \times 10^{-5}$	0
$s = 0{\cdot}3$, $\delta = \frac{1}{30}$	0	$8{\cdot}717 \times 10^{-4}$	$5{\cdot}748 \times 10^{-4}$	$5{\cdot}748 \times 10^{-4}$	$8{\cdot}716 \times 10^{-4}$	0
$h = 0{\cdot}2$, $\delta = -\frac{1}{2}$	0	$8{\cdot}306 \times 10^{-4}$	$3{\cdot}589 \times 10^{-3}$	$3{\cdot}589 \times 10^{-3}$	$8{\cdot}306 \times 10^{-4}$	0

methods have been obtained by us. For $s = 1$ and $h = 0{\cdot}2$ the PH scheme gives on average an error 37% smaller than the error of the FEM schemes and 81% smaller than the error of the FDM implicit schemes. For $s = 0{\cdot}41$ and $h = 0{\cdot}2$ the PH scheme gives on average an error 65% smaller than the error of the FDM and COMP schemes and 99% smaller than the error of the explicit schemes. However, in all cases, as h decreases to 0·1, the average error of our scheme is about 100% smaller than the corresponding error of all other implicit and explicit methods.

Table V. Comparison of the accuracy of our PH scheme with that of other implicit and explicit schemes subject to the Dirichlet boundary conditions (41) at $s = 1$ and 0·41

Method	δ, β	RMS ($h = 0{\cdot}2$)	RMS ($h = 0{\cdot}1$)	RMS ($h = 0{\cdot}05$)	r
Implicit schemes at $s = 1$ and $t = 12{\cdot}5$ with $t_{init} = 4{\cdot}5$					
FDM-4TH*	$\delta = 0$, $\beta_-(\gamma = 1)$	2·367	0·1246	0·008129	3·9
FEM-4TH*	$\delta = \frac{1}{6}$, $\beta_+(\gamma = 1)$	1·395	0·09269	0·005912	4·0
FDM-4TH*	$\delta = 0$, $\beta_-(\gamma = 0)$	0·2393	0·01526	0·001053	3·9
FEM-4TH*	$\delta = \frac{1}{6}$, $\beta_+(\gamma = 0)$	0·2393	0·01522	0·000897	4·1
COMP	$\delta = \frac{1}{12}$, $\beta = 0{\cdot}5$	0·239287	0·015235	0·000974	3·9
PH	$\delta = -\frac{1}{6}$	0·154849	0·001036	0·000018	5·8
PH	$\delta = -\frac{1}{2}$	0·146756	0·001271	0·000021	5·9
Implicit and explicit schemes at $s = 0{\cdot}41$ and $t = 9$ with $t_{init} = 2$					
FTCS* exp.		1·2440	0·30230	0·07550	2·0
3L-4TH* exp.	$\gamma = 1$	0·073470	0·02290	0·001400	4·0
FDM-4TH* imp.	$\delta = 0$, $\beta_-(\gamma = 0)$	0·03718	0·002407	0·000206	3·5
COMP	$\delta = \frac{1}{12}$, $\beta = 0{\cdot}5$	0·03585	0·002378	0·0000150	4·1
PH imp.	$\delta = -\frac{1}{30}$	0·009774	0·000077	0·0000011	6·0
PH imp.	$\delta = -\frac{1}{6}$	0·006532	0·000112	0·0000016	6·1
PH imp.	$\delta = -\frac{1}{2}$	0·020433	0·000274	0·0000030	6·5

Now we consider the solution of the diffusion equation (1) in the interval $0{\cdot}1 \leqslant x \leqslant 1$ with initial value

$$u(x) = 2x + 4\cos(0{\cdot}5x\pi) \quad \text{at } t = 0 \tag{45}$$

and subject to Neumann and Dirichlet boundary conditions which are given respectively by

$$\frac{\partial u}{\partial x} = g(t) = 2 - 2\pi \sin(0{\cdot}05\pi)\mathrm{e}^{-\alpha(\pi/2)^2 t} \quad \text{at } x = 0{\cdot}1 \tag{46}$$

and $u = 2$ at $x = 1$. The exact solution of the problem,

$$u_{\mathrm{ex}} = 2x + 4\cos(0{\cdot}5\pi x)\mathrm{e}^{-\alpha(\pi/2)^2 t}, \tag{47}$$

will be used for the calculation of the RMS error of the numerical solution. Numerical solutions of the above problem have been obtained with our scheme by applying the algebraic expressions (36) and (40a) successively for the implementation of the Neumann boundary condition (46). The exact solution (47) has been used to provide the initial solution at $t = 5{\cdot}2$. The variations in $u(x, t)$ along the rod at $t = 5{\cdot}2$ and $12{\cdot}8$ are shown in Figure 2.

The results for the accuracy of our scheme combined with the corresponding second- and fourth-order boundary condition formulae (36) and (40a) are given in Tables VI and VII respectively. The RMS errors have been calculated for grids with $h = 0{\cdot}05625$, $0{\cdot}1125$ and $0{\cdot}225$ at $t = 15{\cdot}325$ and for the indicated values of the parameters s and δ. We observe that for each value of h the variation in the RMS error as s decreases is very small. It is clear that as s increases to values larger than $S(\delta)$ for a specific value of δ, the induced instabilities of the solutions are much stronger than the corresponding instabilities in the case of Dirichlet boundary conditions. However, the most important conclusion arising from Tables VI and VII is the dramatic reduction in the error of the numerical solution, which is due to the application of our fourth-order formula (40a) for the Neumann boundary condition.

The error distributions $(u - u_{\mathrm{ex}})_i^n$ of our method combined with the boundary condition formulae (36) and (40a) are given in Table VIII at $t = 15{\cdot}325$ for $s = 1$ and $\delta = -\frac{1}{2}$. Clearly, upon applying the expression (40a), we obtain a more evenly distributed truncation error than that obtained by applying the expression (36).

Finally, in Table IX the accuracy of our scheme combined successively with the boundary formulae (36) and (40a) is compared with that of the aforementioned implicit and explicit schemes. The results have been obtained with the initial condition given by the exact solution (47) at $t = 5{\cdot}2$ and $0{\cdot}8$ for comparison reasons and in order to avoid errors in implementing the initial

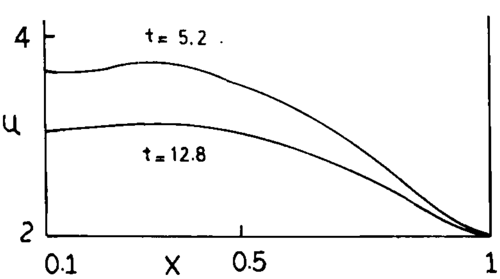

Figure 2. Variation in $u(x)$ subject to Neumann and Dirichlet boundary conditions $u'_x(0{\cdot}1, t) = g(t)$ (equation (46)) and $u(1, t) = 2$ °C respectively at $t = 5{\cdot}2$ and $12{\cdot}8$

Table VI. Estimation of the accuracy of our method subject to the Neumann boundary condition (46) with the formula (36) of order $O(h^2)$ at $t = 15{\cdot}325$

s	δ	RMS ($h = 0{\cdot}225$)	RMS ($h = 0{\cdot}1125$)	RMS ($h = 0{\cdot}05625$)	r
$\frac{1}{6}$	$\frac{1}{30}$	0·00277887	0·00062989	$0{\cdot}1512582 \times 10^{-3}$	2·0
	$-\frac{1}{30}$	0·00277920	0·00062990	$0{\cdot}1512583 \times 10^{-3}$	2·0
	$-\frac{1}{6}$	0·00277994	0·00062991	$0{\cdot}1512584 \times 10^{-3}$	2·0
	$-\frac{1}{2}$	0·00278193	0·00062993	$0{\cdot}1512588 \times 10^{-3}$	2·0
	-1	0·00278403	0·00062997	$0{\cdot}1512593 \times 10^{-3}$	2·0
0·3	$\frac{1}{30}$	0·00263299	0·00063573	$0{\cdot}1509789 \times 10^{-3}$	2·0
	$-\frac{1}{30}$	0·00263365	0·00063572	$0{\cdot}1509787 \times 10^{-3}$	2·0
	$-\frac{1}{6}$	0·00263223	0·00063571	$0{\cdot}1509785 \times 10^{-3}$	2·0
	$-\frac{1}{2}$	0·00262860	0·00063566	$0{\cdot}1509778 \times 10^{-3}$	2·0
	-1	0·00262530	0·00063559	$0{\cdot}1509768 \times 10^{-3}$	2·0
0·5	$\frac{1}{30}$	0·00269564	0·00070591	$0{\cdot}3767557 \times 10$	−1·24
	$-\frac{1}{30}$	0·00273437	0·00062258	$0{\cdot}1512538 \times 10^{-3}$	2·0
	$-\frac{1}{6}$	0·00274923	0·00062207	$0{\cdot}1512528 \times 10^{-3}$	2·0
	$-\frac{1}{2}$	0·00273624	0·00062185	$0{\cdot}1512496 \times 10^{-3}$	2·0
	-1	0·00271905	0·00062148	$0{\cdot}1512446 \times 10^{-3}$	2·0
1·0	$\frac{1}{30}$	0·00256303	0·00238894	$0{\cdot}4576342 \times 10^{4}$	−20·8
	$-\frac{1}{30}$	0·00252853	0·00086052	$0{\cdot}2909138 \times 10$	−15·0
	$-\frac{1}{6}$	0·00247875	0·00061606	$0{\cdot}8958980 \times 10^{-2}$	−3·9
	$-\frac{1}{2}$	0·00240957	0·00063866	$0{\cdot}1512088 \times 10^{-3}$	2·0
	-1	0·00236161	0·00063876	$0{\cdot}1511779 \times 10^{-3}$	2·0

Table VII. Estimation of the accuracy of our method subject to the Neumann boundary condition (46) with our formula (40a) of order $O(h^4)$ at $t = 15{\cdot}325$

s	δ	RMS ($h = 0{\cdot}225$)	RMS ($h = 0{\cdot}1125$)	RMS ($h = 0{\cdot}05625$)	r
$\frac{1}{6}$	$\frac{1}{30}$	$0{\cdot}165876 \times 10^{-4}$	$0{\cdot}994155 \times 10^{-6}$	$0{\cdot}600231 \times 10^{-7}$	4·0
	$-\frac{1}{30}$	$0{\cdot}162884 \times 10^{-4}$	$0{\cdot}989668 \times 10^{-6}$	$0{\cdot}599539 \times 10^{-7}$	4·0
	$-\frac{1}{6}$	$0{\cdot}156553 \times 10^{-4}$	$0{\cdot}980555 \times 10^{-6}$	$0{\cdot}598148 \times 10^{-7}$	4·0
	$-\frac{1}{2}$	$0{\cdot}140132 \times 10^{-4}$	$0{\cdot}956944 \times 10^{-6}$	$0{\cdot}594641 \times 10^{-7}$	4·0
	-1	$0{\cdot}121604 \times 10^{-4}$	$0{\cdot}919308 \times 10^{-6}$	$0{\cdot}589290 \times 10^{-7}$	4·0
0·3	$\frac{1}{30}$	$0{\cdot}196157 \times 10^{-4}$	$0{\cdot}104160 \times 10^{-5}$	$0{\cdot}605916 \times 10^{-7}$	4·1
	$-\frac{1}{30}$	$0{\cdot}201324 \times 10^{-4}$	$0{\cdot}104971 \times 10^{-5}$	$0{\cdot}607171 \times 10^{-7}$	4·1
	$-\frac{1}{6}$	$0{\cdot}213097 \times 10^{-4}$	$0{\cdot}106625 \times 10^{-5}$	$0{\cdot}609687 \times 10^{-7}$	4·1
	$-\frac{1}{2}$	$0{\cdot}244916 \times 10^{-4}$	$0{\cdot}110945 \times 10^{-5}$	$0{\cdot}616046 \times 10^{-7}$	4·2
	-1	$0{\cdot}283345 \times 10^{-4}$	$0{\cdot}117931 \times 10^{-5}$	$0{\cdot}625774 \times 10^{-7}$	4·2
0·5	$\frac{1}{30}$	$0{\cdot}269205 \times 10^{-4}$	$0{\cdot}121158 \times 10^{-5}$	$0{\cdot}255485 \times 10^{-2}$	−11
	$-\frac{1}{30}$	$0{\cdot}345528 \times 10^{-4}$	$0{\cdot}127991 \times 10^{-5}$	$0{\cdot}642762 \times 10^{-7}$	4·4
	$-\frac{1}{6}$	$0{\cdot}417189 \times 10^{-4}$	$0{\cdot}136676 \times 10^{-5}$	$0{\cdot}655519 \times 10^{-7}$	4·4
	$-\frac{1}{2}$	$0{\cdot}589444 \times 10^{-4}$	$0{\cdot}159325 \times 10^{-5}$	$0{\cdot}687880 \times 10^{-7}$	4·5
	-1	$0{\cdot}779329 \times 10^{-4}$	$0{\cdot}196093 \times 10^{-5}$	$0{\cdot}737659 \times 10^{-7}$	4·7
1·0	$\frac{1}{30}$	$0{\cdot}959651 \times 10^{-6}$	$0{\cdot}524021 \times 10^{-5}$	4·024087	−19·5
	$-\frac{1}{30}$	0·000071	$0{\cdot}331457 \times 10^{-5}$	0·021447	−1·2
	$-\frac{1}{6}$	0·000161	$0{\cdot}374454 \times 10^{-5}$	$0{\cdot}495437 \times 10^{-5}$	−0·4
	$-\frac{1}{2}$	0·000288	$0{\cdot}491311 \times 10^{-5}$	$0{\cdot}118564 \times 10^{-6}$	5·4
	-1	0·000377	$0{\cdot}672503 \times 10^{-5}$	$0{\cdot}143286 + 10^{-6}$	5·5

Table VIII. Error distribution $(u - u_{ex})_i$ of our solution subject to the Neumann boundary condition (46) with the formulae (36) and (40a) at $t = 15{\cdot}325$

Method and boundary conditions	h	$x = 0{\cdot}1$	0·325	0·550	0·775	1
PH + (36)	0·05625	$0{\cdot}342 \times 10^{-3}$	$0{\cdot}1170 \times 10^{-3}$	$0{\cdot}7643 \times 10^{-4}$	$0{\cdot}2561 \times 10^{-4}$	0
$s = 1$	0·1125	$0{\cdot}134 \times 10^{-2}$	$0{\cdot}6909 \times 10^{-3}$	$0{\cdot}2981 \times 10^{-3}$	$0{\cdot}9910 \times 10^{-4}$	0
$\delta = -\frac{1}{2}$	0·225	$0{\cdot}456 \times 0^{-2}$	$0{\cdot}2718 \times 10^{-2}$	$0{\cdot}8618 \times 10^{-3}$	$0{\cdot}1847 \times 10^{-3}$	0
PH + (40a)	0·05625	$-0{\cdot}219 \times 10^{-6}$	$-0{\cdot}1487 \times 10^{-6}$	$-0{\cdot}9056 \times 10^{-7}$	$-0{\cdot}4253 \times 10^{-7}$	0
$s = 1$	0·1125	$-0{\cdot}773 \times 10^{-5}$	$-0{\cdot}6283 \times 10^{-5}$	$-0{\cdot}4442 \times 10^{-5}$	$-0{\cdot}2301 \times 10^{-5}$	0
$\delta = -\frac{1}{2}$	0·225	$-0{\cdot}415 \times 10^{-3}$	$-0{\cdot}3774 \times 10^{-3}$	$-0{\cdot}2795 \times 10^{-3}$	$-0{\cdot}1483 \times 10^{-3}$	0

condition. For $s = 1$ and $h = 0{\cdot}225$ the PH scheme in conjuction with the formula (36) gives on average an error 80% smaller than the error of the FMD implicit schemes and 7% larger than the error of the COMP scheme. However, our scheme with the formula (40a) instead of (36) produces an error 100% smaller than the average error of all other methods. For the same parameters and using the boundary formula (40a), our scheme gives a truncation error 49% smaller than the error produced by the corresponding COMP scheme. This error becomes smaller by about 86% at $h = 0{\cdot}1125$ and 96% at $h = 0{\cdot}05265$ than the corresponding errors produced by the COMP method. Similar results are obtained for $s = 0{\cdot}3$.

Table IX. Comparison of the accuracy of our PH scheme with that of other implicit and explicit schemes subject to the Neumann boundary condition (46) with the formulae (36) and (40a) at $s = 1$ and 0·3

Method	δ, β	RMS ($h = 0{\cdot}225$)	RMS ($h = 0{\cdot}1125$)	RMS ($h = 0{\cdot}05625$)	r
Implicit schemes at $s = 1$ and $t = 15$ with $t_{init} = 5{\cdot}2$					
FDM-4TH*	$\delta = 0, \beta_{-}(\gamma = 1)$	0·01478	0·00539	0·00141	1·9
FDM-4TH*	$\delta = 0, \beta_{-}(\gamma = 0)$	0·00912	0·00233	0·00053	2·1
COMP + (36)	$\delta = \frac{1}{12}, \beta = 0{\cdot}5$	0·002261	0·0006133	0·0001547	1·9
COMP + (40a)	$\delta = \frac{1}{12}, \beta = 0{\cdot}5$	0·000569	0·0000352	0·0000022	3·9
PH + (36)	$\delta = -\frac{1}{2}$	0·002409	0·0006386	0·0001512	2·0
PH + (36)	$\delta = -1$	0·0023616	0·0006387	0·0001511	2·0
PH + (40a)	$\delta = -\frac{1}{2}$	0·000288	0·000005	0·0000001	5·4
PH + (40a)	$\delta = -1$	0·000377	0·000006	0·0000001	5·5
Implicit and explicit schemes at $s = 0{\cdot}3$ and $t = 9$ with $t_{init} = 0{\cdot}8$					
FTCS*		0·001753	0·0004235	0·0001064	2·0
3L-4TH*		0·004244	0·0009142	0·0002144	2·1
COMP + (36)	$\delta = \frac{1}{12}, \beta = 0{\cdot}5$	0·002659	0·0006455	0·0001514	2·0
COMP + (40a)	$\delta = \frac{1}{12}, \beta = 0{\cdot}5$	0·000036	0·0000023	0·00000014	4·0
PH + (36)	$\delta = -\frac{1}{6}$	0·0026712	0·0006467	0·0001515	2·0
PH + (36)	$\delta = -\frac{1}{2}$	0·0026673	0·0006466	0·0001515	2·0
PH + (40a)	$\delta = -\frac{1}{6}$	0·000022	0·0000011	0·00000006	4·1
PH + (40a)	$\delta = -\frac{1}{2}$	0·000026	0·0000015	0·00000006	4·2

It is obvious that the incorporation of a discretized formula of low accuracy for the implementation of a Neumann boundary condition drastically reduces the effectiveness of an otherwise highly accurate numerical method. However, our highly improved boundary condition formula (40a) in conjunction with our numerical scheme yields highly accurate solutions with truncation errors of order $O(h^6)$.

The generalization of our numerical method and of our formula for the Neumann boundary condition to the solution of convection-dominated and multidimensional problems will be presented in a series of forthcoming papers.

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