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ON THE TREATMENT OF TIME-DEPENDENT BOUNDARY CONDITIONS IN SPLITTING METHODS FOR PARABOLIC DIFFERENTIAL EQUATIONS

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SUMMARY

Splitting methods for time-dependent partial differential equations usually exhibit a drop in accuracy if boundary conditions become time-dependent. This phenomenon is investigated for a class of splitting methods for two-space dimensional parabolic partial differential equations. A boundary-value correction discussed in a paper by Fairweather and Mitchell for the Laplace equation with Dirichlet conditions, is generalized for a wide class of initial boundary-value problems. A numerical comparison is made for the ADI method of Peaceman–Rachford and the LOD method of Yanenko applied to problems with Dirichlet boundary conditions and non-Dirichlet boundary conditions.

INTRODUCTION

Fairweather and Mitchell[4] investigated alternating direction implicit (ADI) methods for the heat conduction equation

$$\frac{\partial U}{\partial t}=\frac{\partial^2 U}{\partial x_1^2}+\frac{\partial^2 U}{\partial x_2^2} \tag{1}$$

in a domain Ω with Dirichlet boundary conditions along the boundary $\partial\Omega$. Among other things, they discussed the classical Peaceman–Rachford ADI method on a square Ω with square meshes of size h, i.e. the scheme

$$\begin{aligned}\left(I-\frac{1}{2}\frac{\tau}{h^2}\partial_{x_1^2}\right)u_{\bar n}&=\left(I+\frac{1}{2}\frac{\tau}{h^2}\partial_{x_2^2}\right)u_n\\ \left(I-\frac{1}{2}\frac{\tau}{h^2}\partial_{x_2^2}\right)u_{n+1}&=\left(I+\frac{1}{2}\frac{\tau}{h^2}\partial_{x_1^2}\right)u_{\bar n}\end{aligned}, \tag{2}$$

where $u_{\bar n}$, u_n and u_{n+1} denote grid functions defined on the grid $\Gamma_h\cup\partial\Gamma_h$ covering $\Omega\cup\partial\Omega$ and where $\partial_{x_i^2}/h^2$ denotes the usual finite difference replacement of $\partial^2/\partial x_i^2$; furthermore, τ is the integration step and u_n, u_{n+1} present numerical approximations to the exact solution values U at times t_n and t_{n+1}, respectively. By defining u_n and u_{n+1} on the set of boundary grid points $\partial\Gamma_h$ by Dirichlet boundary conditions, the scheme (2) can be applied in all internal grid points provided $u_{\bar n}$ is prescribed along those parts of the boundary for which the x_1-co-ordinate is constant. Peaceman and Rachford defined in their paper[6]

$$u_{\bar n}=U(t_n+\tfrac{1}{2}\tau, x_1, x_2), \qquad (x_1,x_2)\in\partial\Gamma_h \tag{3}$$

D'Yakonov[3] (see also Reference 10, Section 2.9) and Fairweather and Mitchell[4] showed, however, that the method will lose accuracy if the boundary conditions become time-dependent.

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In order to improve the accuracy, Fairweather and Mitchell proposed to replace $u_{\bar{n}}$ along the vertical parts of the boundary by

$$u_{\bar{n}}^* = \frac{U(t_n, x_1, x_2) + U(t_{n+1}, x_1, x_2)}{2} + \frac{\tau}{4h^2}\, \partial_{x_2^2}[U(t_n, x_1, x_2) - U(t_{n+1}, x_1, x_2)] \tag{4}$$

The effect of the modification (4) is that, at points adjacent to a vertical boundary, (2) becomes an $O(h^2 + \tau^2)$ approximation to the equation (1), whereas (3) yields an $O(h^2 + \tau^2/h^2)$ approximation.

The purpose of this paper is to derive the Fairweather–Mitchell modification for a family of splitting methods (including the classical ADI and LOD schemes) and for a rather general class of initial boundary-value problems given by

$$\begin{aligned} &\frac{\partial U}{\partial t} = G_1\left(t, x_1, x_2, U, \frac{\partial U}{\partial x_1}, \frac{\partial^2 U}{\partial x_1^2}\right) + G_2\left(t, x_1, x_2, U, \frac{\partial U}{\partial x_2}, \frac{\partial^2 U}{\partial x_2^2}\right), \qquad (x_1, x_2) \in \Omega \cup \partial\Omega \\ &U(t_0, x_1, x_2) = U_0(x_1, x_2), \qquad (x_1, x_2) \in \Omega \cup \partial\Omega \end{aligned} \tag{5a}$$

$$a_0(t, x_1, x_2)U + a_1(t, x_1, x_2)\frac{\partial U}{\partial x_1} + a_2(t, x_1, x_2)\frac{\partial U}{\partial x_2} = a_3(t, x_1, x_2) \qquad (x_1, x_2) \in \partial\Omega. \tag{5b}$$

Throughout the paper it is assumed that Ω is a bounded and path-connected region in the (x_1, x_2)-space. Further, it is assumed that the functions G_1, G_2 and a_i, $i = 0,1,2,3$, as well as the solution U, are sufficiently smooth.

Since the Fairweather–Mitchell modification has to do with the *time-discretization* of (5), and is not part of the space-discretization, we follow in our analysis the *method of lines* which more or less separates the discretization of $\partial U/\partial t$ from the discretization of the right-hand side of the partial differential equation. In the method of lines we assume that (i) the region $\Omega \cup \partial\Omega$ is replaced by a grid $\Gamma_h \cup \partial\Gamma_h$ characterized by the parameter h and which is defined for each $h \in (0, \bar{h}]$ such that $\Gamma_h \cup \partial\Gamma_h$ is dense in $\Omega \cup \partial\Omega$ as $h \to 0$; (ii) the right-hand side of the partial differential equation and the boundary condition in (5) is discretized on $\Gamma_h \cup \partial\Gamma_h$ in such a way that the equation and the boundary condition together convert into a system of ordinary differential equations

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y + b), \qquad b(t) = g(t, y(t)). \tag{6}$$

Here, to each grid point $\in \Gamma_h \cup \partial\Gamma_h$ there corresponds a component of y, f and b, those of y and f being zero at all boundary grid points $\in \partial\Gamma_h$ and those of b being zero at all internal grid points $\in \Gamma_h$. Thus, y, f and b have as many components as there are grid points in $\Gamma_h \cup \partial\Gamma_h$. Furthermore, system (6) has as many non-trivial equations as there are internal grid points. The function $g(t, y)$ expresses the boundary values in terms of t and y. We shall assume that f is defined for each $h \in (0, \bar{h}]$ and that the exact solution $y(t)$ of (6) and the grid function $U_h(t)$, obtained by restricting the exact solution $U(t, x_1, x_2)$ of the initial boundary-value problem to the grid $\Gamma_h \cup \partial\Gamma_h$, satisfy the condition

$$U_h(t) - [y(t) + b(t)] = \varepsilon(t, h) \to 0 \qquad \text{as } h \to 0 \tag{7}$$

(provided of course that $U_h(t_0) = y(t_0) + b(t_0)$). It should be noted that our assumption on the existence of f for $0 < h \leq \bar{h}$ does not mean that f remains bounded as $h \to 0$. Only for sufficiently smooth grid functions (e.g. $U_h(t)$) the right-hand side functions will converge as $h \to 0$. This observation turns out to be crucial in deriving the Fairweather–Mitchell correction for the problem (5).

LINEAR SPLITTING METHODS

Suppose that we have split the vector function f in (6) according to

$$f(t, y+b)=f_1(t, y+b)+f_2(t, y+b), \qquad b=g(t, y) \tag{8}$$

in which, for example, f_1 and f_2 are assumed to be the approximations for the operators G_1 and G_2 on the grid Γ_h. In terms of f_1 and f_2, we may then define the following family of two-stage splitting formulae[8]

$$\begin{aligned} y_{\bar{n}} &= y_n+\lambda_1\tau f_1(t_n+\alpha_1\tau, y_n+b_n)+\lambda_2\tau f_1(t_n+\alpha_2\tau, y_{\bar{n}}+b_{\bar{n}}^*)+\lambda_3\tau f_2(t_n+\alpha_3\tau, y_n+b_n), \\ y_{n+1} &= y_n+\mu_1\tau f_1(t_n+\alpha_1\tau, y_n+b_n)+(1-\mu_1)\tau f_1(t_n+\alpha_2\tau, y_{\bar{n}}+b_{\bar{n}}^*) \\ &\quad +\mu_2\tau f_2(t_n+\alpha_3\tau, y_n+b_n)+(1-\mu_2)\tau f_2(t_n+\alpha_4\tau, y_{n+1}+b_{n+1}). \end{aligned} \tag{9}$$

The vectors y_n and y_{n+1} denote the numerical approximations to the exact solution $y(t)$ at the step points t_n and $t_{n+1}=t_n+\tau$, respectively. The result $y_{\bar{n}}$ is to be considered as intermediate. The boundary vectors b_n and b_{n+1} are defined by $g(t_n, y_n)$ and $g(t_{n+1}, y_{n+1})$, respectively; $b_{\bar{n}}^*$ is usually defined by (cf. (3))

$$b_{\bar{n}}^* = b_{\bar{n}} = g(t_n+\alpha\tau, y_{\bar{n}}) \tag{10}$$

with an appropriate value of α. The definition of the $b_{\bar{n}}^*$ is often of great importance for the accuracy behaviour of the integration formula. In particular, if g is not constant (10) usually delivers inaccurate results. In this paper we concentrate on the problem how to express $b_{\bar{n}}^*$ in terms of y_n and y_{n+1} so that inaccuracies due to boundary conditions are minimized. We always assume that $b_{\bar{n}}^*$ vanishes at the internal grid Γ_h.

Formula (9) contains a number of two-stage splitting formulae known in the literature. For future reference, in Table I we summarize a few important formulae by specifying the

Table I

Splitting formulae	λ_1	λ_2	λ_3	μ_1	μ_2	α_1	α_2	α_3	α_4	α	p
Peaceman–Rachford[6]	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	—	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	2
Fast form Peaceman–Rachford[8]	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	—	$\frac{1}{2}$	0	1	$\frac{1}{2}$	2
LOD of Yanenko[10]	0	1	0	0	0	—	1	—	1	1	1
Douglas–Rachford[1]	0	1	1	0	0	—	1	0	1	1	1
Douglas–Rachford[2]	$\frac{1}{2}$	$\frac{1}{2}$	1	$\frac{1}{2}$	$\frac{1}{2}$	0	1	0	1	1	2

parameters λ_j, μ_j, α_j, α and the corresponding order of consistency p (cf. Reference 8). It may be observed that the family of splitting formulae (9) is such that the evaluation of y_{n+1} only requires the computation of $f_2(t_n+\alpha_4\tau, y_{n+1}+b_{n+1})$. This aspect should be taken into account when implementing (9) on a computer (cf. Reference 9, and the section on 'The Modification of Fairweather and Mitchell').

The error of approximation

To get insight into the accuracy of the approximation (9) with respect to the definition of $b_{\bar{n}}^*$, we investigate the error of approximation of (9). In the literature one sometimes defines an error of approximation both for the formula yielding $y_{\bar{n}}$ and for the formula yielding y_{n+1} (e.g. Samarskii[7]), but usually the error of approximation is defined for y_{n+1} ignoring the intermediate grid function $y_{\bar{n}}$ (e.g. References 4 and 5). We follow this second approach, i.e. we first eliminate $y_{\bar{n}}$ from (9) by expressing it in terms of $y_n + b_n$ and $y_{n+1} + b_{n+1}$. For notational convenience these grid functions will be denoted by u_n and u_{n+1}, respectively. From (9) it is immediate that

$$y_{\bar{n}} = \nu_1 y_n + (1-\nu_1) y_{n+1} + \nu_2 \tau f_1(t_n + \alpha_1 \tau, u_n) + \nu_3 \tau f_2(t_n + \alpha_3 \tau, u_n) + \nu_4 \tau f_2(t_n + \alpha_4 \tau, u_{n+1}) \quad (11)$$

where

$$\nu_1 = \frac{1-\mu_1-\lambda_2}{1-\mu_1}, \qquad \nu_2 = \frac{\lambda_1 - \lambda_1\mu_1 - \lambda_2\mu_1}{1-\mu_1},$$

$$\nu_3 = \frac{\lambda_3 - \lambda_3\mu_1 - \lambda_2\mu_2}{1-\mu_1}, \qquad \nu_4 = -\lambda_2 \frac{1-\mu_2}{1-\mu_1}.$$

Substitution into the second stage of (9) yields a representation of (9) without the non-step result $y_{\bar{n}}$, i.e.

$$\begin{aligned} y_{n+1} = y_n &+ \tau\mu_1 f_1(t_n + \alpha_1\tau, u_n) + \tau\mu_2 f_2(t_n + \alpha_3\tau, u_n) + \tau(1-\mu_1) f_1(t_n + \alpha_2\tau, \nu_1 u_n \\ &+ (1-\nu_1) u_{n+1} + \tau Y_{\bar{n}} + \tau B_{\bar{n}}) + \tau(1-\mu_2) f_2(t_n + \alpha_4\tau, u_{n+1}) \end{aligned} \quad (12)$$

where $Y_{\bar{n}}$ and $B_{\bar{n}}$ are grid functions defined by

$$Y_{\bar{n}} = \nu_2 f_1(t_n + \alpha_1\tau, u_n) + \nu_3 f_2(t_n + \alpha_3\tau, u_n) + \nu_4 f_2(t_n + \alpha_4\tau, u_{n+1}), \quad (13)$$

$$B_{\bar{n}} = \tau^{-1}(b_{\bar{n}}^* - \nu_1 b_n - (1-\nu_1) b_{n+1}). \quad (14)$$

Note that $Y_{\bar{n}}$ and $B_{\bar{n}}$ vanish at $\partial\Gamma_h$ and Γ_h, respectively.

Equation (12) should approximate the differential equation

$$\frac{dy}{dt} - f(t, u) = 0, \qquad u(t) = y(t) + b(t) = y(t) + g(t, y(t)), \quad (15)$$

or equivalently, the solution y of (15) should satisfy (12) to a sufficient degree of accuracy. By substituting y into (12) we obtain

$$\begin{aligned} &\frac{y(t_{n+1}) - y(t_n)}{\tau} - \mu_1 f_1(t_n + \alpha_1\tau, u(t_n)) - \mu_2 f_2(t_n + \alpha_3\tau, u(t_n)) - (1-\mu_2) f_2(t_n + \alpha_4\tau, u(t_{n+1})) \\ &\qquad - (1-\mu_1) f_1(t_n + \alpha_2\tau, \nu_1 u(t_n) + (1-\nu_1) u(t_{n+1}) + \tau(\tilde{Y}_{\bar{n}} + \tilde{B}_{\bar{n}})) = A_n \end{aligned} \quad (12')$$

where

$$\tilde{Y}_{\bar{n}} = \nu_2 f_1(t_n + \alpha_1\tau, u(t_n)) + \nu_3 f_2(t_n + \alpha_3\tau, u(t_n)) + \nu_4 f_2(t_n + \alpha_4\tau, u(t_{n+1})), \quad (13')$$

$$\tilde{B}_{\bar{n}} = \tau^{-1}(\tilde{b}_{\bar{n}}^* - \nu_1 b(t_n) - (1-\nu_1) b(t_{n+1})), \quad (14')$$

$\tilde{b}_{\bar{n}}^*$ being the grid function obtained by substituting the exact solution $y(t)$ into $b_{\bar{n}}^*$. A_n is the term by which y fails to satisfy equation (12). It will be called the *error of approximation* and is a function of both τ and h.

Firstly, we consider A_n for fixed values of h. By Taylor expansions around the point $(t_{n+1/2}, u(t_{n+1/2}))$ we easily find, for $\tau \to 0$,

$$\begin{aligned} A_n = &\frac{dy}{dt}(t_{n+1/2}) - f(t_{n+1/2}, u(t_{n+1/2})) + (1-\mu_1)\frac{\partial f_1}{\partial u}(t_{n+1/2}, u(t_{n+1/2}))(\tilde{Y}_{\bar{n}} + \tilde{B}_{\bar{n}}) O(\tau) \\ &+ (\tfrac{1}{2} - \alpha_2 - \mu_1\alpha_1 + \mu_1\alpha_2) O(\tau) + (\tfrac{1}{2} - \mu_1 - \nu_1 + \mu_1\nu_1) O(\tau) \\ &+ (\tfrac{1}{2} - \alpha_4 - \mu_2\alpha_3 + \mu_2\alpha_4) O(\tau) + (\tfrac{1}{2} - \mu_2) O(\tau) + O(\tau^2). \end{aligned} \quad (16)$$

From this expression it follows that we always have first-order accuracy in time, provided that $\tilde{B}_{\tilde{n}} = O(1)$ as $\tau \to 0$, i.e. if

$$\tilde{b}^*_{\tilde{n}} = \nu_1 b(t_n) + (1-\nu_1) b(t_{n+1}) + O(\tau) \tag{17}$$

Second-order accuracy in time is obtained if ($\mu_1 \neq 1$)

$$\begin{gathered} \tilde{b}^*_{\tilde{n}} = \nu_1 b(t_n) + (1-\nu_1) b(t_{n+1}) + O(\tau^2) \\ \nu_2 = 0, \qquad \nu_3 + \nu_4 = 0 \end{gathered} \tag{18}$$

and if all coefficients of the remaining terms in (16) vanish. From the theory of numerical integration of ordinary differential equations it follows that the error $y_n - y(t_n)$ also is of order $p = 1$ and $p = 2$ in τ, respectively. Hence, by virtue of our assumption (7), we have

$$U_h(t_n) - u_n = \varepsilon(t_n, h) + c(t_n, h, \tau)\tau^p \tag{19}$$

where the 'error constant' $c(t_n, h, \tau)$ is bounded as $\tau \to 0$.

Next we consider A_n in (12′) for fixed τ and $h \to 0$. The behaviour of A_n for $h \to 0$ is reflected into the behaviour of the error constant c in (19), i.e. if A_n is large for small h the error constant c will also be large, which results in an inaccurate time integration. A minimal requirement is that A_n should be uniformly bounded as $h \to 0$. This requires the uniform boundedness with h of the functions f_1 and f_2 for the arguments occurring in (12′). As already observed in the Introduction, the right-hand side function f, and consequently the split functions f_1 and f_2, only converge as $h \to 0$ if sufficiently smooth argument functions are submitted. Inspection of (12′) reveals that the only argument function which is not yet completely defined is the grid function $\tilde{Y}_{\tilde{n}} + \tilde{B}_{\tilde{n}}$. This function contains the not yet determined grid function $\tilde{b}^*_{\tilde{n}}$ so that the behaviour of A_n as $h \to 0$ will be affected by the choice of $b^*_{\tilde{n}}$. Evidently, $b^*_{\tilde{n}}$ should be chosen such that $\tilde{Y}_{\tilde{n}} + \tilde{B}_{\tilde{n}}$, as defined by (13′) and (14′), becomes on the grid $\Gamma_h \cup \partial\Gamma_h$ a smooth grid function. Thus, it is natural to require that $B_{\tilde{n}}$ is defined by the same difference formulae as $Y_{\tilde{n}}$. This observation leads us to a formula for a boundary-value correction which is an extension of the Fairweather–Mitchell formula (4). Let us derive this formula. Denote

$$\begin{aligned} f_1^{(P)}(t, u) &= G_1^{(P)}\left(t, x_1, x_2, u, \frac{1}{h}\partial_{x_1} u, \frac{1}{h^2}\partial_{x_1^2} u\right) \\ f_2^{(P)}(t, u) &= G_2^{(P)}\left(t, x_1, x_2, u, \frac{1}{h}\partial_{x_2} u, \frac{1}{h^2}\partial_{x_2^2} u\right) \end{aligned} \tag{20}$$

where P runs through Γ_h and where the operators $h^{-1}\partial_{x_i}$ and $h^{-2}\partial_{x_i^2}$ denote numerical approximations to the differential operators $\partial/\partial x_i$ and $\partial^2/\partial x_i^2$ defined at all points $P \in \Gamma_h$ for all grid functions given on the (not necessarily uniform) grid $\Gamma_h \cup \partial\Gamma_h$.

Substitution of (20) into (13′) yields, for $\tilde{Y}^{(P)}_{\tilde{n}}$, the expression

$$\begin{aligned} \tilde{Y}^{(P)}_{\tilde{n}} = {} & \nu_2 G_1^{(P)}\left(t_n + \alpha_1\tau, x_1, x_2, u(t_n), \frac{1}{h}\partial_{x_1} u(t_n), \frac{1}{h^2}\partial_{x_1^2} u(t_n)\right) \\ & + \nu_3 G_2^{(P)}\left(t_n + \alpha_3\tau, x_1, x_2, u(t_n), \frac{1}{h}\partial_{x_2} u(t_n), \frac{1}{h^2}\partial_{x_2^2} u(t_n)\right) \\ & + \nu_4 G_2^{(P)}\left(t_n + \alpha_4\tau, x_1, x_2, u(t_{n+1}), \frac{1}{h}\partial_{x_2} u(t_{n+1}), \frac{1}{h^2}\partial_{x_2^2} u(t_{n+1})\right) \end{aligned} \tag{21}$$

for all $P \in \Gamma_h$. Suppose now that we extend the definition of the difference operators $h^{-1}\partial_{x_i}$ and $h^{-2}\partial_{x_i^2}$ to boundary points $P \in \partial\Gamma_h$ for all grid functions given on the grid $\Gamma_h \cup \partial\Gamma_h$. Then it is easily verified that by the choice

$$
\begin{aligned}
b_{\tilde{n}}^{*(P)} = {} & \nu_1 b_n^{(P)} + (1-\nu_1) b_{n+1}^{(P)} + \nu_2 \tau G_1^{(P)}\left(t_n + \alpha_1\tau,\, x_1,\, x_2,\, u_n,\, \frac{1}{h}\partial_{x_1} u_n\, \frac{1}{h^2}\partial_{x_1^2} u_n\right) \\
& + \nu_3 \tau G_2^{(P)}\left(t_n + \alpha_3\tau,\, x_1,\, x_2,\, u_n,\, \frac{1}{h}\partial_{x_2} u_n,\, \frac{1}{h^2}\partial_{x_2^2} u_n\right) \\
& + \nu_4 \tau G_2^{(P)}\left(t_n + \alpha_4\tau,\, x_1, x_2,\, u_{n+1},\, \frac{1}{h}\partial_{x_2} u_{n+1},\, \frac{1}{h^2}\partial_{x_2^2} u_{n+1}\right)
\end{aligned}
\tag{22}
$$

$\tilde{B}_{\tilde{n}}^{(P)}$ is given by the same expression as the right-hand side of (21). We shall call (22) the *Fairweather–Mitchell correction.* The effect of this correction is an equal degree of smoothness of the grid function $\tilde{Y}_{\tilde{n}} + \tilde{B}_{\tilde{n}}$ in all points of the grid $\Gamma_h \cup \partial\Gamma_h$.

Example. The formula given by (22) presents nothing more than an extension of the Fairweather–Mitchell formula (4) to a general class of splitting formulae and a general class of initial boundary-value problems. To see this we consider the special problem (1) analysed by Fairweather and Mitchell, although we do not restrict the boundary conditions to those of Dirichlet type but admit a general boundary function $b = g(t, y)$.

By substituting the Peaceman–Rachford parameters of Table I into (9) and putting for all P from the uniform square grid Γ_h

$$f_i^{(P)}(t, u) = h^{-2}(\partial_{x_i^2} u)^{(P)},$$

we retain scheme (2). Next, we substitute these parameters into (22) and observe that $f_i^{(P)} = G_i^{(P)}$ to obtain the formula

$$b_{\tilde{n}}^{*(E)} = \tfrac{1}{2}(u_n^{(E)} + u_{n+1}^{(E)}) + \frac{\tau}{4h^2}[(\partial_{x_2^2} u_n)^{(E)} - (\partial_{x_2^2 n+1})^{(E)}],\ E \in \partial\Gamma_h. \tag{22'}$$

This formula is defined as soon as $\partial_{x_2^2}$ is specified along the boundary. A closer examination reveals that in this case of a square region $b_{\tilde{n}}^*$ is only needed along the vertical parts of the boundary and therefore $\partial_{x_2^2}$ needs only definition along these boundary parts. Formula (22′) thus transforms into

$$b_{\tilde{n}}^{*(E)} = \tfrac{1}{2}(b_n^{(E)} + b_{n+1}^{(E)}) + \frac{\tau}{4h^2}[(\partial_{x_2^2} b_n)^{(E)} - (\partial_{x_2^2} b_{n+1})^{(E)}]. \tag{22''}$$

In the special case of Dirichlet conditions this formula is seen to be identical to the Fairweather–Mitchell formula (4). In general, the grid functions b_n and b_{n+1} are obtained by discretizing the boundary conditions. For instance, in the case of (5b) a first-order discretization yields (see Figure 1)

$$b^{(E)} = g^{(E)}(t, y) = (1 + a_0^{(E)})(2y^{(P)} - y^{(W)}) + a_1^{(E)} \frac{y^{(P)} - y^{(W)}}{h} + a_2^{(E)} \frac{y^{(N)} - y^{(S)}}{2h} - a_3^{(E)} \qquad \square$$

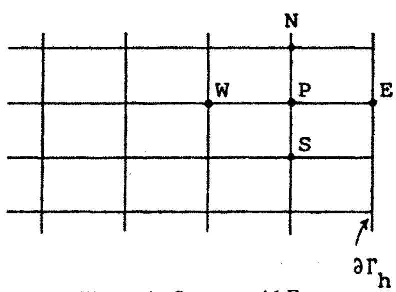

Figure 1. Square grid Γ_h

The *derivation* of formula (22) is purely formal. Its *evaluation* is another matter because it requires the *a priori* knowledge of $u_{n+1}^{(P)}$, $(\partial_{x_2}u_{n+1})^{(P)}$ and $(\partial_{x_2^2}u_{n+1})^{(P)}$ at boundary points, which, in general, depend on the new approximation y_{n+1}. Even in case of Dirichlet boundary conditions, when $b(t)=g(t)$, it depends on the type of region Ω whether $(\partial_{x_2}u_{n+1})^{(P)}$ and $(\partial_{x_2^2}u_{b+1})^{(P)}$ can be evaluated at the beginning of the integration step. In most cases the introduction of the Fairweather–Mitchell modification (22) will induce a coupling between the equation for y_n and y_{n+1}, and consequently additional computational effort to solve the implicit equations.

THE ADI METHOD OF PEACEMAN AND RACHFORD

For a furter illustration of the treatment of time-dependent boundary conditions we shall apply the Fairweather–Mitchell modification to the ADI method of Peaceman and Rachford and perform a number of numerical experiments. In the section on 'The Lod Method of Yanenko', the same experiments will be performed. For convenience of testing we now restrict ourselves to problems of type (5) on the unit square and assume a uniform Γ_h. We consider the Peaceman–Rachford method in the so-called Varga form,[9] i.e.

$$\begin{aligned} y_{\tilde{n}} &= y_n+\tfrac{1}{2}\tau f_1(t_n+\tfrac{1}{2}\tau,\ y_{\tilde{n}}+b_{\tilde{n}}^*)+\tfrac{1}{2}\tau f_2(t_n+\tfrac{1}{2}\tau,\ y_n+b_n) \\ y_{n+1} &= 2y_{\tilde{n}}-y_n+\tfrac{1}{2}\tau f_2(t_n+\tfrac{1}{2}\tau,\ y_{n+1}+b_{n+1})-\tfrac{1}{2}\tau f_2(t_n+\tfrac{1}{2}\tau,\ y_n+b_n), \end{aligned} \tag{23}$$

where, for $P\in\Gamma_h$, $f_i^{(P)}(t,u)$ is given in (20) with ∂_{x_i} and $\partial_{x_i^2}$ the standard finite difference operators. The precise form of the boundary function $b(t)=g(t,y(t))$ will be given later.

The modification of Fairweather and Mitchell

From (22) the modification of Fairweather and Mitchell is seen to be given by

$$\begin{aligned} b_{\tilde{n}}^{*(P)} &= \tfrac{1}{2}b_n^{(P)}+\tfrac{1}{2}b_{n+1}^{(P)}+\tfrac{1}{4}\tau G_2^{(P)}\left(t_n+\frac{1}{2}\tau,\ x_1,\ x_2,\ u_n,\ \frac{1}{h}\partial_{x_2}u_n,\ \frac{1}{h^2}\partial_{x_2^2}u_n\right) \\ &\quad -\tfrac{1}{4}\tau G_2^{(P)}\left(t_n+\frac{1}{2}\tau,\ x_1,\ x_2,\ u_{n+1},\ \frac{1}{h}\partial_{x_2}u_{n+1},\ \frac{1}{2}\partial_{x_2^2}u_{n+1}\right), \end{aligned} \tag{24}$$

for $P\in\partial\Gamma_h$. For constant boundary values b we have $b_{\tilde{n}}^{*(P)}=b$ for all $P\in\partial\Gamma_h$, where (24) is applied. Note that for the fast-form method this depends on the occurrence of the time t in the differential operator $G_2(\alpha_1\neq\alpha_2)$. As already observed at the end of the section on 'Linear Splitting Methods', in most cases expression (24) cannot be evaluated in an explicit way. Let us distinguish between Dirichlet conditions and non-Dirichlet conditions. For Dirichlet conditions the evaluation of (24) is easy to perform in our case of the unit square. If Ω has a more general form, say Ω is an L-shaped region, the computational procedure has to be reorganized (see Reference 4). In the case of Dirichlet conditions, however, it is always possible to replace the finite difference operators by the corresponding differential operators. When doing this, the computational procedure need not be reorganized in order to implement (24) for different types of regions. For Dirichlet problems we implemented two algorithms: (i) algorithm (23) with $b_{\tilde{n}}^*=g(t_n+\frac{1}{2}\tau)$ (in the tables of results denoted by PR), and (ii) algorithm (23) using the modification (24) (in the tables of results denoted by FMPR).

In case of non-Dirichlet conditions, (24) couples the y_n – and y_{n+1} – level at internal grid points in the neighbourhood of vertical boundaries. Hence, the modification of Fairweather and Mitchell then requires the solution of large systems of equations with a special sparsity pattern. From a computational point of view this is unattractive, as the classical Peaceman–Rachford scheme only requires the solution of systems of (nonlinear) equations with a tridiagonal Jacobian matrix. For non-Dirichlet problems we also implemented two algorithms: (i) The PR algorithm, i.e. (23) with $b_{\bar{n}}^* = g(t_n + \frac{1}{2}\tau, y_{\bar{n}})$, and (ii) the PR algorithm followed by another application of (23) on the same initial vector y_n, but now with $b_{\bar{n}}^*$ defined according to (24) (in the tables of results denoted by IFMPR). The IFMPR algorithm, defined in this way, can be interpreted as a first iteration step to solve the coupled problem just mentioned.

Numerical experiments

To demonstrate experimentally the effect of the modification (24), several experiments were performed. These consist of solving the heat equation

$$\frac{\partial U}{\partial t} = \mathrm{d}\,(t)\left\{\frac{\partial^2 U}{\partial x_1^2} + \frac{\partial^2 U}{\partial x_2^2}\right\} + \left(\frac{\partial U}{\partial x_1}\right)^{\nu} + \left(\frac{\partial U}{\partial x_2}\right)^{\nu} + v(t, x_1, x_2) \tag{25}$$

in the cylinder $[0 \leq t \leq 1] \times \Omega$, Ω being the unit square in the (x_1, x_2)-plane. A splitting of $v = \frac{1}{2}v + \frac{1}{2}v$ was used in all experiments.

Two types of boundary conditions were considered, viz. conditions of the first kind ($a_1 = a_2 = 0$ in (5b)) and of the second kind ($a_0 = 0$ in (5b)). In both cases the same test-set was used.

For all examples used, the exact solution is known. The boundary conditions as well as the initial condition follow from the exact solution. The test examples are based on equation (25) with the parameters given in Table II.

Table II

Example Number	Solution $U(t, x_1, x_2)$	Diffusion coefficient $\mathrm{d}(t)$	Non-linearity parameter ν	Inhomogeneous term $v(t, x_1, x_2)$
1	$1 + e^{-t}(x_1^2 + x_2^2)$	1	0	$-e^{-t}(x_1^2 + x_2^2 + 4) - 2$
2	$1 + e^{-t}(x_1^3 + x_2^3)$	1	0	$-e^{-t}(x_1^3 + x_2^3 + 6x_1 + 6x_2) - 2$
3	$1 + (x_1^2 - x_2^2)/(1+t)$	$1/(1+t)$	0	$-(x_1^2 - x_2^2)/(1+t)^2 - 2$
4	$1 + \sin(2\pi t) \sin(x_1 x_2)$	1	0	$\sin(x_1 x_2)\{2\pi\cos(2\pi t) + \sin(2\pi t)(x_1^2 + x_2^2)\} - 2$
5	$1 + e^{-t}(x_1^2 + x_2^2)$	$1/(1+t)$	2	$-e^{-t}(x_1^2 + x_2^2 + 4/(1+t) + 4e^{-t}(x_1^2 + x_2^2))$

Concerning the implementation, we remark that all experiments were carried out for a sequence of constant step-sizes τ, viz. $\frac{1}{5}$, $\frac{1}{10}$, $\frac{1}{20}$ and $\frac{1}{40}$.

All examples were semi-discretized using finite differences. At internal grid-points we used second-order, symmetrical differences, while the boundary condition of the second kind was replaced by a second-order, three-point difference relation. The grid-size h runs through the same range of values as τ does.

The tridiagonal Jacobian matrices, used to solve the implicit equations by means of a Newton-type process, were numerically evaluated using forward differences. In case of constant partial derivatives $\partial f/\partial y$, these matrices were determined once; in all other cases they were updated every integration step. In the constant case the implicit equations were solved with one Newton iteration; otherwise we performed two Newton iterations.

Finally, to measure the accuracy obtained we define

$$\mathrm{sd} = -{}^{10}\log\,(\text{maximum absolute error at } t = 1).$$

Table III. sd-values in the case of boundary conditions of the first kind

		Example 1		Example 2		Example 3		Example 4		Example 5	
h	τ	PR	FMPR	PR	FMPR	PR	FMPR	PR	FMPR	PR	FMPR
	$\frac{1}{5}$	2·18	3·24	2·00	3·04	2·67	4·29	1·37	2·00	2·13	2·13
	$\frac{1}{10}$	2·80	3·86	2·62	3·66	3·28	5·22	2·18	2·51	2·75	3·51
$\frac{1}{5}$	$\frac{1}{20}$	3·40	4·46	3·23	4·26	3·89	5·97	2·88	3·10	3·36	4·11
	$\frac{1}{40}$	4·01	5·07	3·83	4·86	4·49	6·63	3·51	3·71	3·96	4·71
	$\frac{1}{5}$	2·07	3·20	1·81	3·03	2·57	3·74	1·18	1·99	1·93	2·84
$\frac{1}{10}$	$\frac{1}{10}$	2·70	3·82	2·46	3·65	3·20	5·03	1·91	2·50	2·62	3·48
	$\frac{1}{20}$	3·30	4·43	3·08	4·25	3·80	5·95	2·66	3·09	3·23	4·09
	$\frac{1}{40}$	3·90	5·03	3·69	4·85	4·40	6·59	3·33	3·69	3·83	4·69
	$\frac{1}{5}$	1·99	3·20	1·70	3·02	2·46	3·28	1·09	1·99	1·79	2·47
$\frac{1}{20}$	$\frac{1}{10}$	2·64	3·82	2·34	3·64	3·14	4·42	1·77	2·49	2·48	3·48
	$\frac{1}{20}$	3·25	4·42	2·98	4·25	3·75	5·77	2·49	3·08	3·14	4·08
	$\frac{1}{40}$	3·85	5·03	3·59	4·85	4·36	6·59	3·21	3·68	3·74	4·68
	$\frac{1}{5}$	1·95	3·20	1·64	3·02	2·40	3·04	1·04	1·99	1·71	2·26
$\frac{1}{40}$	$\frac{1}{10}$	2·57	3·82	2·25	3·64	3·04	3·92	1·70	2·49	2·36	3·19
	$\frac{1}{20}$	3·23	4·42	2·90	4·24	3·72	5·07	2·36	3·08	3·05	4·08
	$\frac{1}{40}$	3·83	5·03	3·52	4·85	4·32	6·47	3·08	3·68	3·68	4·68

The results, in terms of the sd values, for the preceding examples with boundary conditions of the first kind are given in Table III. Table IV contains the results for the five examples with a Dirichlet condition on $\{(x_1, x_2)|(x_1 = 0, 0 < x_2 < 1) \cup (0 \leqslant x_1 \leqslant 1, x_2 = 0) \cup (0 \leqslant x_1 \leqslant 1, x_2 = 1)\}$ and a von Neumann condition on $\{(x_1, x_2)|(x_1 = 1, 0 < x_2 < 1\}$.

Observation of the results of Tables III and IV leads us to the following conclusions:

1. When the space-discretization error is negligible with respect to the time-integration error, the accuracy of the classical Peaceman–Rachford method (PR) decreases when τ is kept fixed and h tends to zero. We also mention that under these conditions the loss of accuracy diminishes. The two asterisks in Table IV indicate numerical instability.

Table IV. sd-values in the case of boundary conditions of the second kind

		Example 1		Example 2		Example 3		Example 4		Example 5	
h	τ	PR	IFMPR	PR	IFMPR	PR	IFMPR	PR	IFMPR	PR	IFMPR
	$\frac{1}{5}$	2·31	3·37	2·12	2·15	2·72	3·57	2·14	2·15	2·39	2·75
$\frac{1}{5}$	$\frac{1}{10}$	2·93	3·88	2·18	2·15	3·33	4·21	2·86	2·58	3·01	3·30
	$\frac{1}{20}$	3·54	4·39	2·16	2·16	3·93	4·98	3·40	3·07	3·62	3·86
	$\frac{1}{40}$	4·14	4·95	2·16	2·16	4·54	5·84	3·77	3·43	4·22	4·43
	$\frac{1}{5}$	2·17	3·24	1·86	2·76	2·59	3·29	1·86	2·14	2·05	2·78
$\frac{1}{10}$	$\frac{1}{10}$	2·80	3·90	2·52	2·62	3·22	3·89	2·62	2·66	2·75	3·35
	$\frac{1}{20}$	3·41	4·43	2·67	2·64	3·82	4·58	3·32	3·20	3·36	3·92
	$\frac{1}{40}$	4·01	5·00	2·65	2·65	4·42	5·32	3·92	3·70	3·97	4·48
	$\frac{1}{5}$	2·08	3·03	1·74	3·13	2·47	3·15	1·73	1·83	1·86	2·33
$\frac{1}{20}$	$\frac{1}{10}$	2·73	3·92	2·38	3·25	3·14	3·73	2·46	2·66	2·56	3·39
	$\frac{1}{20}$	3·35	4·47	3·02	3·19	3·76	4·37	3·13	3·27	3·33	3·96
	$\frac{1}{40}$	3·91	5·05	3·22	3·19	4·36	5·04	3·77	3·83	3·83	4·54
	$\frac{1}{5}$	2·03	2·95	1·68	2·88	2·40	1·99	1·67	1·71	*	*
$\frac{1}{40}$	$\frac{1}{10}$	2·66	3·85	2·28	3·56	3·04	3·65	2·38	2·46	2·42	3·07
	$\frac{1}{20}$	3·31	4·49	2·93	3·80	3·72	4·27	3·05	3·18	3·12	3·99
	$\frac{1}{40}$	3·91	5·08	3·56	3·77	4·32	4·90	3·67	3·88	3·72	4·58

2. In the case of *Dirichlet conditions*, the Fairweather–Mitchell modification (FMPR) is less sensitive for decreasing values of h, again for fixed τ. An exception must be made for example 3, where for large values of τ a reduction of h causes a significant loss of accuracy. For boundary conditions of the *second kind* the modification (IFMPR) remains sensitive for decreasing values of h. This is due to the fact that the error of approximation of the algorithm IFMPR still contains the term h^{-2}.
3. In the case of boundary conditions of the first kind, FMPR is superior to PR, because the computational work of FMPR is hardly more than that of PR. However, in the case of boundary conditions of the second kind, IFMPR requires approximately twice as many computations or, in other words, the PR method can be applied with half the step-length for the same amount of computational work. Consequently, if we let h fixed and if the time-integration error dominates, we then expect a reduction of the error of the second-order algorithm PR by a factor 4 or, equivalently, an increase of its sd-value by approximately $^{10}\log 4 \simeq 0{\cdot}6$. Therefore, IFMPR is more efficient than PR if their sd-values differ by more than 0·6. With exception of examples 2 and 4, IFMPR generally improves the accuracy is such a way that it can be called 'competitive'.

THE LOD METHOD OF YANENKO

We repeated the experiments of the preceding section for the LOD method (see Table I).

$$\begin{aligned} y_{\tilde{n}} &= y_n + \tau f_1(t_n + \tau, y_{\tilde{n}} + b^*_{\tilde{n}}), \\ y_{n+1} &= y_{\tilde{n}} + \tau f_2(t_n + \tau, y_{n+1} + b_{n+1}). \end{aligned} \tag{26}$$

The definition of Γ_h, and of the components of the vector functions f_i, $i = 1,2$, and $b = g(t, y)$ is as in the earlier section on 'The ADI Method of Peaceman and Rachford'.

The modification of Fairweather and Mitchell

From (22) the boundary-value modification is immediately found to be

$$b^{*(P)}_{\tilde{n}} = b^{(P)}_{n+1} - \tau G^{(P)}_2\left(t_n + \tau, x_1, x_2, u_{n+1}, \frac{1}{h}\,\partial_{x_2} u_{n+1}, \frac{1}{h^2}\,\partial_{x_2^2} u_{n+1}\right), \tag{27}$$

for $P \in \partial\Gamma_h$. It is of importance to observe that even in case of a constant boundary value b the modified boundary values $b^{*(P)}_{\tilde{n}}$ usually are not equal to b. In this case we have

$$b^{*(P)}_{\tilde{n}} = b - \tau G_2(t_n + \tau, x_1^{(P)}, x_2^{(P)}, b, 0, 0).$$

Consequently, if the modification is not applied and if the boundary values are constant it may pay to define the operator G_2 in such a way, if possible, that $b^{*(P)}_{\tilde{n}} = b$. It shall be clear that with respect to the evaluation and implementation of formula (27), all remarks made in the preceding section apply to the LOD method.

For problems with boundary conditions of the first kind we again implemented two algorithms: (i) (26) with $b^*_{\tilde{n}} = g(t_n + \tau)$, i.e. the classical algorithm (in the tables of results denoted by YA), and (ii) (26) using the boundary-value modification (27) (in the tables of results denoted by FMYA).

For problems with boundary conditions of the second kind we implemented (i) the YA algorithm with $b^*_{\tilde{n}}$ defined by $g(t_n + \tau, y_{\tilde{n}})$, i.e. the classical algorithm, and (ii) the algorithm consisting of one application of the classical one followed by another application of the YA algorithm on the same initial vector y_n, but now with $b^*_{\tilde{n}}$ defined according to (27) (in the tables of results denoted by IFMYA).

Table V. sd-values in the case of boundary conditions of the first kind

		Example 1		Example 2		Example 3		Example 4		Example 5	
h	τ	YA	FMYA	YA	FMYA	YA	FMYA	YA	FMYA	YA	FMYA
	$\frac{1}{5}$	1·95	2·45	1·46	2·31	1·30	2·53	1·02	1·73	1·61	1·72
$\frac{1}{5}$	$\frac{1}{10}$	2·10	2·63	1·60	2·49	1·51	2·79	1·19	2·00	1·79	1·94
	$\frac{1}{20}$	2·31	2·85	1·80	2·71	1·76	3·04	1·40	2·28	2·02	2·20
	$\frac{1}{40}$	2·55	3·11	2·04	2·97	2·03	3·32	1·65	2·56	2·29	2·47
	$\frac{1}{5}$	1·83	2·42	1·32	2·29	1·22	2·53	0·96	1·72	1·46	1·71
$\frac{1}{10}$	$\frac{1}{10}$	1·97	2·60	1·45	2·47	1·42	2·78	1·11	2·00	1·63	1·93
	$\frac{1}{20}$	2·16	2·83	1·64	2·69	1·66	3·04	1·30	2·28	1·86	2·19
	$\frac{1}{40}$	2·39	3·09	1·87	2·95	1·93	3·31	1·53	2·56	2·12	2·46
	$\frac{1}{5}$	1·77	2·42	1·25	2·29	1·19	2·52	0·93	1·72	1·39	1·70
$\frac{1}{20}$	$\frac{1}{10}$	1·90	2·60	1·38	2·47	1·38	2·77	1·06	2·00	1·55	1·93
	$\frac{1}{20}$	2·09	2·83	1·57	2·69	1·61	3·03	1·24	2·28	1·78	2·18
	$\frac{1}{40}$	2·32	3·08	1·79	2·94	1·88	3·30	1·46	2·56	2·04	2·45
	$\frac{1}{5}$	1·74	2·42	1·22	2·29	1·17	2·52	0·91	1·72	1·35	1·70
$\frac{1}{40}$	$\frac{1}{10}$	1·87	2·60	1·35	2·47	1·35	2·77	1·04	2·00	1·52	1·93
	$\frac{1}{20}$	2·05	2·83	1·53	2·69	1·59	3·03	1·22	2·27	1·74	2·18
	$\frac{1}{40}$	2·28	3·08	1·75	2·94	1·86	3·30	1·43	2·55	2·01	2·45

Numerical experiments

All algorithms were applied to the examples listed earlier in 'Numerical Experiments', using the same values of τ and h, as well as the same finite difference formulae. The treatment of the implicit equations was also unchanged. The results obtained for boundary conditions of the first kind are given in Table V. Table VI contains the results obtained for conditions of the second kind.

Table VI. sd-values in the case of boundary conditions of the second kind

		Example 1		Example 2		Example 3		Example 4		Example 5	
h	τ	YA	IFMYA	YA	IFMYA	YA	IFMYA	YA	IFMYA	YA	IFMYA
	$\frac{1}{5}$	2·38	2·62	1·56	2·06	1·43	2·39	1·06	1·11	1·92	1·63
$\frac{1}{5}$	$\frac{1}{10}$	2·59	2·72	1·69	2·85	1·64	3·03	1·31	1·39	2·16	1·82
	$\frac{1}{20}$	2·83	2·89	1·87	2·43	1·89	3·06	1·57	1·69	2·41	2·01
	$\frac{1}{40}$	3·09	3·07	2·09	2·20	2·16	3·23	1·85	2·01	2·68	2·20
	$\frac{1}{5}$	2·23	2·49	1·45	1·58	1·34	2·07	1·01	1·04	1·88	1·74
$\frac{1}{10}$	$\frac{1}{10}$	2·42	2·80	1·59	1·80	1·53	2·57	1·25	1·30	2·11	1·96
	$\frac{1}{20}$	2·65	2·96	1·77	2·11	1·77	3·23	1·51	1·58	2·35	2·15
	$\frac{1}{40}$	2·91	3·17	1·99	2·65	2·04	3·39	1·79	1·89	2·62	2·36
	$\frac{1}{5}$	2·15	2·27	1·40	1·44	1·29	1·95	0·99	1·00	1·87	1·81
$\frac{1}{20}$	$\frac{1}{10}$	2·33	2·50	1·53	1·61	1·48	2·36	1·22	1·25	2·10	2·04
	$\frac{1}{20}$	2·56	2·78	1·71	1·85	1·72	2·81	1·48	1·52	2·34	2·26
	$\frac{1}{40}$	2·81	3·12	1·92	2·16	1·99	3·25	1·75	1·81	2·61	2·48
	$\frac{1}{5}$	2·11	2·18	1·38	1·38	1·27	1·89	0·98	0·98	1·87	*
$\frac{1}{40}$	$\frac{1}{10}$	2·29	2·38	1·50	1·54	1·46	2·27	1·21	1·22	2·05	2·08
	$\frac{1}{20}$	2·51	2·63	1·68	1·76	1·69	2·66	1·46	1·48	2·28	2·32
	$\frac{1}{40}$	2·77	2·92	1·89	2·02	1·96	3·02	1·74	1·76	2·54	2·56

The results of Tables V and VI justify the following conclusions:

1. When the time-integration error dominates, the accuracy of the locally one-dimensional method (YA) decreases with h for fixed τ. The loss of accuracy, however, diminishes. The asterisk in Table VI indicates numerical instability.
2. In the case of *Dirichlet conditions* the scheme with the Fairweather–Mitchell modification (FMYA) does not exhibit a loss of accuracy if h becomes small and τ is kept fixed. For boundary conditions of the *second kind* the situation is different. In a lot of cases the accuracy of the modified scheme (IFMYA) decreases with h for fixed τ (cf. conclusion (2) in the preceding section). It also happens, however, that the results become better if h becomes small (see example 5, where the space discretization error is equal to zero).
3. Because of the fact that, for Dirichlet conditions, the computational effort of the modified scheme (FMYA) is hardly more than that of the unmodified one (YA), it certainly pays to apply the Fairweather–Mitchell correction in the case of boundary conditions of the first kind. For boundary conditions of the second kind our results indicate that the Fairweather–Mitchell correction applied to the locally one-dimensional method is of less practical value.

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