stichting
mathematisch
centrum

MC

AFDELING NUMERIEKE WISKUNDE
(DEPARTMENT OF NUMERICAL MATHEMATICS)

NW 55/78 APRIL

P.J. VAN DER HOUWEN & J.G. VERWER

ONE-STEP SPLITTING METHODS FORMULATED FOR SEMI-DISCRETE PARABOLIC EQUATIONS

Preprint

2e boerhaavestraat 49 amsterdam

Printed at the Mathematical Centre, 49, 2e Boerhaavestraat, Amsterdam.

The Mathematical Centre, founded the 11-th of February 1946, is a non-profit institution aiming at the promotion of pure mathematics and its applications. It is sponsored by the Netherlands Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O).

AMS(MOS)subject classification scheme: 65L05, 65M05, M20

One-step splitting methods formulated for semi-discrete parabolic equations *)

by

P.J. van der Houwen & J.G. Verwer

ABSTRACT

The main purpose of the paper is to discuss splitting methods for parabolic equations via the method of lines. Firstly, we deal with the formulation of these methods for semi-discrete equations

$$\frac{dy}{dt} = f(y), \quad f \text{ non-linear},$$

f satisfying a linear splitting relation $f(y) = \sum_{i=1}^{k} f_i(y)$. A class of one-step integration formulas is defined, which is shown to contain all known splitting methods, provided the functions f_i are defined appropriately. For a number of methods stability results are given. Secondly, attention is paid to alternating direction methods for problems with an arbitrary non-linear coupling between space derivatives. Numerical results of these methods are compared with results obtained by a hopscotch method.

KEYWORDS & PHRASES: *Numerical analysis, Ordinary differential equations, Partial differential equations, Method of lines, Splitting methods*

---

*) This report will be submitted for publication elsewhere

1. INTRODUCTION

A flexible approach in the numerical solution of time-dependent partial differential equations is obtained by applying the so-called *method of lines*. Herewith the numerical solution process may be considered as to consist of two parts, viz. semi-discretization and time-integration. In the *semi-discretization* the partial differential equation is converted into a system of ordinary differential equations by discretizing the space variables, while the time variable is left continuous. Usually, the semi-discretization is obtained, either by the finite difference method [14], or by the finite element method [6]. In the *time-integration* the resulting system of ordinary differential equations is integrated by a numerical integration method [11] to obtain an approximate solution of the original differential equation. If the discretizations of the space variable(s) and the time variable are considered as if they were performed simultaneously, the solution of the time-dependent partial differential equation is said to be approximated via the so-called *direct grid* approach.

Both approaches are essentially the same, i.e. every method obtained via the lines approach may in the end be considered as a direct grid method, and both are followed in literature. A difference is lying in the *presentation* and *formulation* of methods. To this purpose the method of lines approach is more suited than the direct approach. It generally leads to a more general formulation and a more unifying treatment of methods for time-dependent equations. It is the purpose of this paper to discuss splitting methods for parabolic equations via the method of lines, and in particular the *time integration*.

In the numerical solution of partial differential equations splitting methods have been introduced to avoid the solution of large and complicated systems of non-linear equations, which arise when applying fully implicit integration formulas to multi-dimensional problems. More generally, the idea of splitting is to break down a complicated (multi-dimensional) process into a series of simple (one-dimensional) processes. The *aim of splitting* is always to obtain a *feasible computational process*. Well-known splitting methods (also referred to as fractional step methods) are the alternating direction methods [2,3,13], the locally one-dimensional methods [19],

and the hopscotch methods [7,8]. In the literature these methods are usually formulated and analyzed as direct grid methods.

We consider the numerical integration of non-linear, semi-discrete parabolic equations of the general type

$$(1.1) \qquad \frac{dy}{dt} = f(y), \quad f: \mathbb{R}^N \to \mathbb{R}^N,$$

where the vector function f can be *linearly split* into k terms, k > 1, i.e.

$$(1.2) \qquad f(y) = \sum_{i=1}^{k} f_i(y), \quad f_i: \mathbb{R}^N \to \mathbb{R}^N.$$

The functions f_i are called *splitting functions* and depend on the original partial differential equation and the type of semi-discretization. In section 2 of this paper, we define a general class of one-step integration formulas for systems (1.1)-(1.2), which we shall call *splitting formulas*. In this definition no a priori knowledge of the function f_i is assumed, except that they define a meaningful splitting, i.e. a splitting which admits a feasible computational process for a certain problem class. In our discussion we thus distinguish between splitting functions and spliting formulas, while a combination of both leads to a *splitting method*. This distinction is an immediate consequence of the method of lines approach, and it shows clearly that a certain type of splitting functions can usually be combined with more than one type of splitting formulas, and vice versa. Several examples of known splitting methods, considered in this way, are discussed in section 3. Because these methods are based on a linear spliting (1.2), we refer to them as *linear splitting methods*. In section 4 we pay attention to splitting methods of the alternating direction type for problems with an arbitrary *non-linear coupling* between space derivatives. For such problems relation (1.2) is too restrictive if one wants to apply alternating direction methods. Some numerical results of these *non-linear splitting methods* are discussed in section 6 and compared with results obtained by a hopscotch method. Section 5 is devoted to a discussion of stability properties of splitting methods. Using matrix theory, results are given for the greater part of the methods discussed in the examples. These results are presented in a uniform way and are based on two basic theorems, viz. a theorem due to KELLOG [12], and a theorem given by WACHSPRESS [18].

In the following, our considerations are restricted to equations in autonomous form. This is done for notational convenience and is not essential, i.e. results can be easily extended to systems of the non-autonomous form

$$\frac{dy}{dt} = f(t,y), \quad f: \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N. \tag{1.3}$$

This paper is based on two institute reports [16], [17]. For the preparation of these reports the book of YANENKO [19] and the survey of GOURLAY [10] were very useful.

2. LINEAR SPLITTING FORMULAS

Consider the m-th stage, one-step integration formula

$$\begin{aligned} y_{n+1}^{(0)} &= y_n, \\ y_{n+1}^{(j)} &= y_n + \tau_n \sum_{\ell=0}^{j} \sum_{i=1}^{k} \lambda_{j\ell i} f_i(y_{n+1}^{(\ell)}), \quad j = 1(1)m, \\ y_{n+1} &= y_{n+1}^{(m)}, \end{aligned} \tag{2.1}$$

where y_n denotes the numerical approximation at $t = t_n$ and $\tau_n = t_{n+1} - t_n$. Each formula from class (2.1) is called a *linear splitting formula*. The parameters $\lambda_{j\ell i}$ serve to make this scheme a consistent and stable approximation to the differential equation (1.1). In particular, however, they should be used to exploit the splitting property (1.2) in order to obtain an attractive computational process. For example, if the Jacobian matrix of each f_i is tridiagonal, they should be chosen in such a way that each intermediate approximation $y_{n+1}^{(j)}$ can be obtained from the solution of a system of non-linear equations with a tridiagonal Jacobian too. In that case Newton iteration is easy to apply.

Observe that if $\lambda_{jji} = 0$, the resulting scheme is explicit. In the theory of splitting methods this case does not occur. Observe that for $k = 1$, i.e. when no splitting is performed, scheme (2.1) reduces to an m-th stage, semi-explicit Runge-Kutta scheme [1]. In most applications the number of stages m equals the number of splitting functions k.

Let $\Phi(\tau_n, y_n, y_{n+1})$ denote the increment function of the one-step formula (2.1), i.e.

$$y_{n+1} = y_n + \tau_n \Phi(\tau_n, y_n, y_{n+1}). \tag{2.2}$$

We employ the following definition of order of consistency:

DEFINITION. The formula is said to be consistent of order p if p is the largest integer for which

$$y(t+\tau) - y(t) - \tau\Phi(\tau, y(t), y(t+\tau)) = O(\tau^{p+1}), \quad \tau \to 0, \tag{2.3}$$

holds, where y(t) denotes a sufficiently differentiable solution to the differential equation.

The consistency conditions can be derived through a formal Taylor expansion of Φ. Splitting formulas are usually of order 1 or 2. Conditions up to order 3 are listed in table 2.1. The derivation of these conditions is straightforward and is given in [16].

We do not give a special convergence proof of (2.1), as convergence results for one-step formulas defined by general increment functions Φ are well known (see e.g. [11] or [15]).

Table 2.1 Consistency conditions for (2.1)

p = 1	$\sum_{\ell=0}^{m} \lambda_{m\ell i} = 1, \quad i = 1(1)k,$
p = 2	$\sum_{\ell=1}^{m} \sum_{r=0}^{\ell} \lambda_{m\ell i}\lambda_{\ell rj} = \frac{1}{2}, \quad i,j = 1(1)k,$
p = 3	$\sum_{r=0}^{\ell} \lambda_{\ell rj} = c_\ell, \quad j = 1(1)k,$
	$\sum_{\ell=1}^{m} \lambda_{m\ell i}\, c_\ell^2 = \frac{1}{3}, \quad i = 1(1)k,$
	$\sum_{\ell=1}^{m} \sum_{r=1}^{\ell} \sum_{s=0}^{r} \lambda_{m\ell i}\lambda_{\ell rj}\lambda_{rst} = \frac{1}{6}, \quad i,j,t = 1(1)k.$

3. SURVEY OF IMPORTANT LINEAR SPLITTING METHODS

In this section we list a number of linear splitting formulas of type (2.1), which all can be associated to splitting methods already given in the literature as direct grid methods.

At this place it should be noted that the treatment of boundary conditions is part of the semi-discretization process. The splitting formulas are defined for systems of ordinary differential equations. The only requirement for those systems is that they admit a linear splitting leading to computational feasibility.

3.1 Two-term splitting methods

Let $k = 2$, i.e. let

$$f(y) = f_1(y) + f_2(y), \tag{3.1}$$

and consider the 2-th stage formula

$$\begin{aligned} y_{n+1}^{(1)} &= y_n + \tau_n[(\lambda-\tfrac{1}{2})f_1(y_n)+\tfrac{1}{2}f_1(y_{n+1}^{(1)})+\lambda f_2(y_n)], \\ y_{n+1} &= y_n + \tau_n[(\frac{2\lambda-1}{2\lambda})f_1(y_n) + \frac{1}{2\lambda} f_1(y_{n+1}^{(1)}) + \\ &\quad + \tfrac{1}{2}f_2(y_n) + \tfrac{1}{2}f_2(y_{n+1})], \end{aligned} \tag{3.2}$$

λ still being a free parameter. It is easily verified that for each splitting (3.1) this formula is second order consistent. This simple formula represents several known splitting methods. We will show this in the following subsections by identifying f_i and substituting special values for the free parameter λ.

3.1.1 Two alternating direction implicit methods

Let Ω denote a bounded and path-connected region in the two-dimensional (x_1,x_2)-space with sides parallel to the coordinate axes. Let $\delta\Omega$ denote the boundary curve of Ω, and consider a parabolic equation of the non-linear type

$$u_t = G_1(x_1,x_2,u,u_{x_1},u_{x_1x_1}) + G_2(x_1,x_2,u,u_{x_2},u_{x_2x_2}) \tag{3.3}$$

defined in the cylinder $\Omega \times [0,T]$. Further, assume the boundary conditions on $\delta\Omega \times [0,T]$ of the form

(3.3') $\quad a(x_1,x_2)u + b(x_1,x_2)u_n = c(x_1,x_2)$, u_n normal derivative.

Superimpose a rectilinear grid on Ω with grid lines parallel to the coordinate axes, and *semi-discretize* equations (3.3)-(3.3') using standard finite differences. This yields a system of ordinary differential equations

(3.4) $\quad \frac{dy}{dt} = f(y)$, f being 5-point coupled.

Each component of y and f is associated to a grid point belonging to the interior of Ω, while a dependency exists only between nearest neighbours along grid lines (see fig.3.1 for an illustrative example).

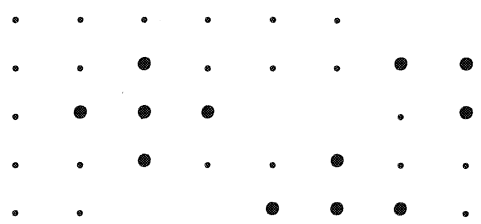

fig.3.1 A set of internal grid points

Next define the functions f_1 and f_2 to be the semi-discretized operators G_1 and G_2. We shall call this splitting

(3.5) $\quad f(y) = f_1(y) + f_2(y)$

of (3.4) the *differential operator splitting*. By substituting these functions into formula (3.2) with $\lambda = \frac{1}{2}$ we obtain an alternating direction implicit method of the type of PEACEMAN & RACHFORD [13]:

$$y_{n+1}^{(1)} = y_n + \tfrac{1}{2}\tau_n[f_1(y_{n+1}^{(1)}) + f_2(y_n)],$$

(3.6)

$$y_{n+1} = y_{n+1}^{(1)} + \tfrac{1}{2}\tau_n[f_1(y_{n+1}^{(1)}) + f_2(y_{n+1})].$$

The choice $\lambda = 1$ then leads to an alternating direction implicit method of the type discussed by DOUGLAS & RACHFORD [3]:

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n + \tau_n[\tfrac{1}{2}f_1(y_n) + \tfrac{1}{2}f_2(y_{n+1}^{(1)}) + f_2(y_n)], \\
y_{n+1} &= y_{n+1}^{(1)} + \tau_n[\tfrac{1}{2}f_2(y_{n+1}) - \tfrac{1}{2}f_2(y_n)].
\end{aligned}
\tag{3.7}
$$

The intermediate approximation $y_{n+1}^{(1)}$ in (3.6) is a first order consistent approximation at the intermediate point $t = t_n+\frac{1}{2}\tau_n$, whereas in (3.7) $y_{n+1}^{(1)}$ is first order consistent at the point $t = t_n+\tau_n$.

Because of the 5-point coupling and the absence of partial derivatives with respect to x_2 in G_1 and x_1 in G_2, the Jacobian matrices of $f_1(y)$ and $f_2(y)$ are *tridiagonal*. This makes the methods computationally attractive. The calculation of $y_{n+1}^{(1)}$ requires the solution of a system of non-linear equations with a tridiagonal Jacobian for each grid line along the x_1-axis. By using a Newton iteration process this calculation is easy to perform. The same holds for the calculation of y_{n+1}, but now for grid lines along the x_2-axis.

3.1.2 The odd-even hopscotch method

Again we consider a 5-*point-coupled* system, but now we assume that the coupling between its components is fully non-linear:

$$\frac{dy}{dt} = f(y), \quad \text{5-point coupling, fully non-linear.} \tag{3.8}$$

Such a system may arise when semi-discretizing a non-linear parabolic equation of the type

$$u_t = G(x_1,x_2,u,u_{x_1},u_{x_2},u_{x_1x_1},u_{x_2x_2}), \tag{3.9}$$

with boundary conditions like (3.3'). For such a system the *linear* alternating direction splitting of the preceding section can not be realized. In section 4 a non-linear alternating direction splitting will be considered which can deal with this type of equation. In the class of linear splitting methods however, it is also possible to deal with (3.8), viz. by hopscotch methods.

As in the preceding section, each component of (3.8) is associated to a grid point of a two-dimensional grid. In our formulation it is now convenient (see also section 4) to introduce vector functions $f_o, f_\bullet, f_+$

and f_x, such that

$$f(y) = f_o(y)+f_\bullet(y)+f_+(y)+f_x(y), \tag{3.10}$$

and similarly for y, which are defined by the PRESCRIPTION: divide the set of grid points into 4 subsets, say $\Omega_o,\Omega_\bullet,\Omega_+$ and Ω_x, as shown in figure 3.2; let the symbol $\wedge$ be generic and let $f_\wedge^{[i]}(y)$ denote the i-th component of $f_\wedge(y)$; then

$$f_\wedge^{[i]}(y) = \begin{cases} f^{[i]}(y), & \text{if corresponding grid point} \in \Omega_\wedge \\ 0, & \text{otherwise.} \end{cases} \tag{3.11}$$

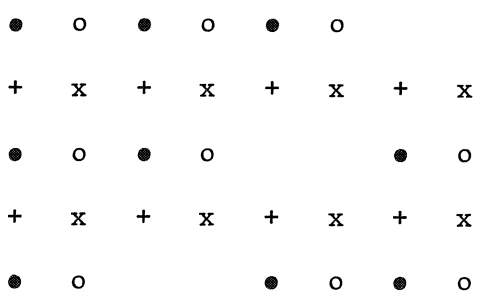

Fig.3.2 Four subsets of gridpoints

Next define the splitting functions f_1 and f_2 for equation (3.8) by

$$\begin{aligned} f_1(y) &= f_o(y)+f_+(y), \\ f_2(y) &= f_\bullet(y)+f_x(y). \end{aligned} \tag{3.12}$$

By substituting these functions into formula (3.2) and putting $\lambda = \frac{1}{2}$ the odd-even hopscotch method is readily recognized. By computing $y_{n+1}^{(1)}$ first at the grid points $\in \Omega_\bullet \cup \Omega_x$, and then at the points $\in \Omega_o \cup \Omega_+$, only *scalar equations* are to be solved. The same holds for y_{n+1} when the computing order is reversed. This property makes the method attractive with respect to computational effort per integration step.

3.1.3 The line hopscotch method

Instead of 5-point coupled systems we now consider 9-*point coupled* ones, and again assume that the components are fully, non-linearly coupled:

(3.13) $\frac{dy}{dt} = f(y)$, 9-point coupling, fully non-linear.

Such systems usually arise by semi-discretizing parabolic equations containing a mixed derivative, i.e. equations of the type

(3.14) $u_t = G(x_1,x_2,u,u_{x_1},u_{x_2},u_{x_1x_1},u_{x_1x_2},u_{x_2x_2})$,

with boundary conditions (3.3'). They may also arise from semi-discretization of equations without a mixed derivative (e.g. (3.9)), viz. by using non-orthogonal grid lines. To nine-point coupled systems the *line-hopscotch method* can be applied [7,8]. Using the notation of the preceding section the corresponding splitting functions f_1 and f_2 read

$$f_1(y) = f_o(y)+f_\bullet(y),$$
$$f_2(y) = f_+(y)+f_x(y). \tag{3.15}$$

By substituting these functions into formula (3.2) and putting $\lambda = \frac{1}{2}$ the line hopscotch method is easily recognized. By computing $y_{n+1}^{(1)}$ first at the grid points $\in \Omega_+ \cup \Omega_x$, and then at the points $\in \Omega_o \cup \Omega_\bullet$, only systems of non-linear equations with a tridiagonal Jacobian matrix are to be solved; the same holds for the computation of y_{n+1}. The function (3.15) define the splitting along horizontal grid lines. In a similar way the splitting may be defined for vertical lined. It is observed that the present method requires half the number of tridiagonal inversions as required by the Peaceman-Rachford method. In addition, it can be applied to fully non-linear equations possessing a 9-point, as well as a 5-point, coupling. These advantages make the method attractive from a computational point of view.

REMARK 3.1. For non-autonomous equations (1.5) and corresponding splittings of the type

(3.1') $f(t,y) = f_1(t,y)+f_2(t,y)$,

formula (3.2) may be reformulated to obtain the second order family

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n+\tau_n[(\lambda-\tfrac{1}{2})f_1(t_n+\alpha\tau_n,y_n) + \\
&\quad + \tfrac{1}{2}f_1(t_n+\beta\tau_n,y_{n+1}^{(1)}) + \lambda f_2(t_n+\gamma\tau_n,y_n)], \qquad (3.2')\\
y_{n+1} &= y_n+\tau_n[(\frac{2\lambda-1}{2\lambda})f_1(t_n+\delta\tau_n,y_n) + \frac{1}{2\lambda}f_1(t_n+\beta\tau_n,y_{n+1}^{(1)}) + \\
&\quad + \tfrac{1}{2}f_2(t_n+\gamma\tau_n,y_n) + \tfrac{1}{2}f_2(t_n+(1-\gamma)\tau_n,y_{n+1})],
\end{aligned}
$$

where the new parameters δ,β must satisfy $(2\delta-1)\lambda + \beta-\delta = 0$ for a given λ. It should be observed that other choices of the time increments are possible.

3.2 Multi-term splitting methods

Consider the k-dimensional, non-linear parabolic equation (see (3.3))

$$
u_t = \sum_{i=1}^{k} G_i(x_1,\ldots,x_k,u,u_{x_i},u_{x_ix_i}) \qquad (3.16)
$$

with boundary conditions of the type given in section 3.1.1. Assume that standard finite differences are applied to obtain the semi-discrete system

$$
\frac{dy}{dt} = f(y),\ f(y) = \sum_{i=1}^{k} f_i(y), \quad (2k+1)\text{-coupling} \qquad (3.17)
$$

where each f_i denotes the semi-discretize operator G_i, i.e. we assume the *differential operator splitting* (see section 3.1.1).

3.2.1 A method of Gourlay and Mitchell

Let k = 3, and consider the three stage formula

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n + \tfrac{1}{2}\tau_n[f_1(y_n)+f_2(y_{n+1}^{(1)})],\\
y_{n+1}^{(2)} &= y_{n+1}^{(1)} + \tfrac{1}{2}\tau_n[f_3(y_{n+1}^{(1)})+f_3(y_{n+1}^{(2)})], \qquad (3.18)\\
y_{n+1} &= y_{n+1}^{(2)} + \tfrac{1}{2}\tau_n[f_2(y_{n+1}^{(2)})+f_1(y_{n+1})].
\end{aligned}
$$

It is easily verified that (3.18) is *second order* consistent. This type of splitting method has been suggested by GOURLAY & MITCHELL [9]. The second stage only contains the function f_3, whereas f_1 and f_2 occur at both the first and the third stage. The method is based, partly on the principle of alternating directions, and partly on the principle of the locally one-dimensional method discussed in the next subsection.

3.2.2 The locally one-dimensional method of Yanenko

Consider the k-th stage formula

$$
\begin{aligned}
&y_{n+1}^{(0)} = y_n, \\
&y_{n+1}^{(j)} = y_{n+1}^{(j-1)} + \tau_n[(1-\alpha)f_j(y_{n+1}^{(j-1)}) + \alpha f_j(y_{n+1}^{(j)})], \quad j = 1(1)k, \qquad (3.19) \\
&y_{n+1} = y_{n+1}^{(k)},
\end{aligned}
$$

where α is still a free parameter. For every α the method is *first order* consistent. This type of splitting method emanates from YANENKO [19]. The method is called locally one-dimensional, because of the fact that at the j-th stage only the semi-discretized one-dimensional operator G_j is used. In applications the free parameter α usally equals $\frac{1}{2}$ or 1.

3.2.3 The method of approximation corrections of Yanenko

Consider the (k+1)-th stage formula

$$
\begin{aligned}
&y_{n+1}^{(0)} = y_n, \\
&y_{n+1}^{(j)} = y_{n+1}^{(j-1)} + \tfrac{1}{2}\tau_n f_j(y_{n+1}^{(j)}), \quad j = 1(1)k, \qquad (3.20) \\
&y_{n+1} = y_n + \tau_n f(y_{n+1}^{(k)}).
\end{aligned}
$$

This type of splitting method also emanates from YANENKO [19], who called it the method of approximation corrections. In the preliminary, locally one-dimensional stages stability (see section 5) is achieved, while the last stage serves to make the method *second order* consistent.

3.2.4 The method of stabilizing corrections of Douglas and Gunn

Consider the k-th stage formula

$$y_{n+1}^{(1)} = y_n + \tau_n[f(y_n) - f_1(y_n) + f_1(y_{n+1}^{(1)}],$$

$$(3.21) \qquad y_{n+1}^{(j)} = y_{n+1}^{(j-1)} + \tau_n[f_j(y_{n+1}^{(j)}) - f_j(y_n)], \quad j = 2(1)k,$$

$$y_{n+1} = y_{n+1}^{(k)}.$$

For $k \leq 3$ this splitting method was introduced by DOUGLAS & RACHFORD [3] and later, in its general form, formulated by DOUGLAS & GUNN [3] (see also YANENKO [19]). At the first stage, a consistent approximation is evaluated, while all succeeding stages serve to improve the stability. Therefore it is called the method of stabilizing corrections. It is only *first order* consistent.

3.2.5 The method of stabilizing corrections of Douglas

Consider the k-th stage formula

$$y_{n+1}^{(1)} = y_n \; \tau_n[f(y_n) - \tfrac{1}{2}f_1(y_n) + \tfrac{1}{2}f_1(y_{n+1}^{(1)})],$$

$$(3.22) \qquad y_{n+1}^{(j)} = y_{n+1}^{(j-1)} + \tfrac{1}{2}\tau_n[f_j(y_{n+1}^{(j)}) - f_j(y_n)], \quad j = 2(1)k,$$

$$y_{n+1} = y_{n+1}^{(k)}.$$

This splitting method is a *second order* analogue of (3.21). For $k = 2$ we obtain the earlier mentioned Douglas-Rachford method (3.7). The case $k = 3$ originates from DOUGLAS [4], whereas the general case has not been discussed in the literature.

4. NON-LINEAR SPLITTING METHODS

In sections (3.1.2) and (3.1.3) we discussed two hopscotch methods for fully non-linear equations (such as (3.9)) with an arbitrary coupling between space derivatives. To these equations alternating direction implicit methods

based on *linear* splitting formulas (such as (3.6),(3.7)) cannot be applied. In this section we introduce *non-linear* splitting formulas and functions, by which alternating direction implicit methods can be defined for fully non-linear equations of the type (3.9). In particular, we give two methods which may be considered as generalizations of (3.6) and (3.7).

We introduce the non-linear function F: $\mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}^N$, F still to be specified, such that

$$f(y) = F(y,y). \tag{4.1}$$

Next we consider the one-parameter class of integration formulas

$$\begin{aligned} y_{n+1}^{(1)} &= y_n + \tau_n[\tfrac{1}{2}F(y_{n+1}^{(1)},y_n) + (\lambda-\tfrac{1}{2})F(y_n,y_n)], \\ y_{n+1} &= y_n + \tau_n[\tfrac{1}{2}F(y_{n+1}^{(1)},y_n) + \frac{2\lambda-1}{2\lambda}F(y_n,y_{n+1}) + \frac{1-\lambda}{2\lambda}F(y_{n+1}^{(1)},y_{n+1})]. \end{aligned} \tag{4.2}$$

Formula (4.2) is a one-step formula of the form (2.2) to which the usual definitions of consistency and convergence apply. A straight-forward Taylor expansion yields that (4.2) is consistent of order p = 2 for every *splitting function* F satisfying (4.1). Observe that this formula is implicit in the first argument of F at the first stage and in the second argument at the second stage.

Now assume for a moment that f(y) can be written as in (3.1), i.e. $f(y) = f_1(y)+f_2(y)$. By defining

$$F(u,v) = f_1(u)+f_2(v) \tag{4.3}$$

and substituting into (4.2), we recover the one-parameter class of linear splitting formulas (3.2), which, in turn, contains the underlying formulas for the alternating direction implicit methods (3.6) and (3.7). Hence, for 5-point coupled equations satisfying a linear differential operator splitting, like (3.5), the $\lambda = \frac{1}{2}$ and $\lambda = 1$ formulas of class (4.2) can immediately be identified with the formulas of Peaceman-Rachford and Douglas-Rachford.

Next, let f(y) be defined by (3.8), i.e. f does not satisfy a linear differential operator splitting. Using the notation of section (3.1.2), we define the function F(u,v) by

$$
\begin{aligned}
(4.4)\qquad F(u,v) = {} & f_o(Du_o+u_\bullet+v_x+(I-D)v_o) + \\
& f_x(Du_x+u_+ +v_o+(I-D)v_x) + \\
& f_\bullet(Du_\bullet+u_o+v_+ +(I-D)v_\bullet) + \\
& f_+(Du_+ +u_x+v_\bullet+(I-D)v_+),
\end{aligned}
$$

where I denotes the unit matrix and D a diagonal matrix whose elements are still free. Let us substitute this function F into formula (4.2). Because of the special character of the function f(y) defined by (3.8), we have that the calculation of $y_{n+1}^{(1)}$ requires the solution of a system of non-linear equations with a tridiagonal Jacobian for each grid line from $\Omega_o \cup \Omega_\bullet$ and $\Omega_+ \cup \Omega_x$, respectively. A similar observation can be made for the calculation of y_{n+1}, but now for grid lines in the other direction. We thus see that (4.2),(4.4) defines a family of alternating direction implicit methods for the *fully non-linear* partial differential equation (3.9). The choice $\lambda = \frac{1}{2}$, i.e.

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n + \tfrac{1}{2}\tau_n F(y_{n+1}^{(1)}, y_n), \\
y_{n+1} &= y_{n+1}^{(1)} + \tfrac{1}{2}\tau_n F(y_{n+1}^{(1)}, y_{n+1}),
\end{aligned}
\qquad (4.5)
$$

is immediately recognized as a method of the *Peaceman-Rachford* type, while the choice $\lambda = 1$, i.e.

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n + \tfrac{1}{2}\tau_n[F(y_{n+1}^{(1)}, y_n) + F(y_n, y_n)], \\
y_{n+1} &= y_{n+1}^{(1)} + \tfrac{1}{2}\tau_n[F(y_n, y_{n+1}) - F(y_n, y_n)],
\end{aligned}
\qquad (4.6)
$$

delivers a *Douglas-Rachford* type method.

A difficulty in the application of these non-linear methods is the choice of the diagonal matrix D, whose elements serve as weight factors for the elements of the main diagonals of the Jacobians of the systems of non-linear equations. The most obvious choice is $D = \frac{1}{2}I$; then the original Peaceman-Rachford splitting is obtained if the original partial equation would be $u_t = u_{x_1x_1} + u_{x_2x_2}$. In other cases, however, e.g. for $u_t = u_{x_1x_1} + \alpha u_{x_2x_2}$,

$\alpha \neq 1$, this choice may lead to instabilities (see section 5).

REMARK 4.1. The idea of non-linear splitting for fully non-linear problems is not restricted to two dimensions. The Douglas formulas (3.22), $k \geq 2$, are easily generalized for k-argument splitting functions $F(y,\ldots,y)$. For example, for $k = 3$ we then obtain

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n + \tfrac{1}{2}\tau_n[F(y_{n+1}^{(1)},y_n,y_n) + F(y_n,y_n,y_n)], \\
y_{n+1}^{(2)} &= y_{n+1}^{(1)} + \tfrac{1}{2}\tau_n[F(y_n,y_{n+1}^{(2)},y_n) - F(y_n,y_n,y_n)], \qquad (4.7) \\
y_{n+1} &= y_{n+1}^{(2)} + \tfrac{1}{2}\tau_n[F(y_n,y_n,y_{n+1}) - F(y_n,y_n,y_n)].
\end{aligned}
$$

For a definition of the splitting function $F(y,y,y)$ in this case, we refer to [17].

REMARK 4.2. For non-autonomous equations $y' = f(t,y)$ and the corresponding splitting $f(t,y) = F(t,y,y)$, formula (4.2) is easily reformulated to obtain the family of second order formulas

$$
\begin{aligned}
y_{n+1}^{(1)} &= y_n + \tau_n[\tfrac{1}{2}F(t_n+\alpha\tau_n,y_{n+1}^{(1)},y_n) + (\lambda-\tfrac{1}{2})F(t_n,y_n,y_n)], \\
y_{n+1} &= y_n + \tau_n[\tfrac{1}{2}F(t_n+\alpha\tau_n,y_{n+1}^{(1)},y_n) + \frac{2\lambda-1}{2\lambda}F(t_n+\tau_n,y_n,y_{n+1}) + \qquad (4.2') \\
&\qquad + \frac{1-\lambda}{2\lambda}F(t_n+(1-\alpha)\tau_n,y_{n+1}^{(1)},y_{n+1}).
\end{aligned}
$$

For a given λ the parameter α must satisfy $(2\lambda-1)\alpha = 0$. For $\lambda \in \{\frac{1}{2},1\}$ and functions F satisfying $F(t,u,v) = f_1(t,u)+f_2(t,v)$, the corresponding formulas belong to family (3.2').

5. STABILITY PROPERTIES

Splitting methods find their interest, next to the computational feasibility, in possessing unconditional stability properties for interesting problem classes. In the direct grid approach such properties are usually investigated by making use of harmonic analyis [14]. In the method of lines approach it is more convenient to make use of matrix theory. In this way

unconditional stability properties can be shown for all splitting formulas previously discussed. These results will be based on two basic theorems, viz. a theorem due to KELLOG [12] and a theorem given in WACHPRESS [18].

5.1 The amplification matrix and the stability function

With respect to stability we confine ourselves to the first order variational equation of the integration formula under consideration. This approach is widely accepted in the literature and has proved to be satisfactory. For our formulas this first order variational equation is always of the form

$$y_{n+1} = A_n y_n, \tag{5.1}$$

A_n denoting the *amplification matrix*. Let us first consider formula (2.1). Then A_n is defined by

$$A_n = R(\tau_n J_1, \ldots, \tau_n J_k), \tag{5.2}$$

where J_i denotes the Jacobian $\partial f_i/\partial y$ at $y = y_n$, and where R is a *matrix-valued* function defined by the formal relations

$$\begin{aligned} &R^{[o]}(Z_1,\ldots,Z_k) = I, \quad I \text{ the unit matrix,} \\ &R^{[j]}(Z_1,\ldots,Z_k) = I + \sum_{\ell=0}^{j} \sum_{i=1}^{k} \lambda_{j\ell i}\, Z_i R^{[\ell]}(Z_1,\ldots,Z_k), \quad j = 1(1)m, \\ &R(Z_1,\ldots,Z_k) = R^{[m]}(Z_1,\ldots,Z_k). \end{aligned} \tag{5.3}$$

This function is completely determined by the splitting formula, and is therefore called the *stability function* of the formula. The value of the stability function, obtained by substituting the Jacobian matrices J_i of the particular problem to be integrated, is the amplification matrix (5.2). Thus, the amplification matrix depends both on the splitting formula and the splitting functions, and therefore on the problem to be integrated. The reader should be aware of the fact that the matrix arguments of R may be non-commuting.

Expressions (5.1)-(5.3) can be obtained in a more direct manner by applying formula (2.1) to the linear equation

$$\frac{dy}{dt} = Jy, \tag{5.4}$$

where

$$J = \sum_{i=1}^{k} J_i. \tag{5.5}$$

In fact, it is usally more convenient to start from the linear equation (5.4). This equation, with additional restrictions on the matrices J_i, is then considered as a *test-model* for stability.

Next we consider the class of non-linear splitting formulas (4.2). As observed in section 4, this class is reduced to class (3.2) if F(v,w) satisfies a linear splitting relation like (4.3). For linear equations (5.4), such a linear relation does always exist. Because (3.2) is a special case of (2.1), it is not necessary to give the stability function of class (4.2) at this place. In this special case the matrices J_i, i = 1,2, should be interpreted as the derivatives $\partial F/\partial v$ and $\partial F/\partial w$, respectively.

5.2. The test-model and two basic theorems

For the derivation of stability criteria one must make assumptions on the matrices J and J_i. Restrictions which are usually imposed are [5]:

(5.6)

1^o The matrices J_i are symmetric and negative definite.

2^o The matrices J_i commute.

To interpret these restrictions, consider the k-dimensional equation

$$u_t = \sum_{i=1}^{k} u_{x_i x_i} \tag{5.7}$$

on the unit cube with zero Dirichlet boundary conditions. If we impose a uniform grid and semi-discretize using standard finite differences, we obtain a linear system of type (5.4). If we further assume the differential operator splitting, i.e. the matrices J_i are associated to the operators $\partial^2/\partial x_i^2$, then properties (5.6) hold.

The linear equation (5.4), whose matrices J_i satisfy conditions (5.6), is usally considered as a test-model for stability. In some situations, however, equations are considered of which the conditions imposed are less

restrictive (see e.g. section 5.3).

For the derivation of the stability criteria - when using matrix theory - it is of importance whether the stability function R is factorized or not. We shall distinguish these two cases and treat them separately.

5.2.1 A useful theorem for factorized stability functions

The following theorem of KELLOG [12] may be used in many cases where we have factorized stability functions:

THEOREM 5.1. *Let* B *be a given matrix. Let* B^T *denote the transposed of* B, *and let* ρ *denote a positive scalar. If* $B + B^T$ *is non-positive definite, then*

a) $\rho I - B$ is non-singular

b) $\|(\rho I - B)^{-1}\|_2 \leq \rho^{-1}$,

c) $\|(\rho I + B)(\rho I - B)^{-1}\|_2 \leq 1$.

Further, if $B + B^T$ *is negative definite, then*

d) $\|(\rho I - B)^{-1}\|_2 < \rho^{-1}$,

e) $\|(\rho I + B)(\rho I - B)^{-1}\|_2 < 1$.

This theorem enables us to obtain stability results of the type

$$\|A_n\|_2 < 1,$$

or

$$\|A^n\|_2 \leq C,\ n \geq 1,\ C \text{ a constant},$$

where A_n and A represent amplification matrices. Further, this theorem can be used to obtain results under less restrictive conditions than imposed by (5.6).

5.2.2 A useful theorem for non-factorized stability functions

The following theorem, given in WACHSPRESS [18], is useful when we have to deal with a non-factorized stability function:

THEOREM 5.2. *Let* B *be a symmetric, negative definite matrix. Let* M *be a non-singular matrix and define* $C = I + \rho M^{-1} B$. *If* $M^T + M + \rho B$ *is positive definite, then the spectral radius* $\sigma(C) < 1$ *for all positive scalars* ρ.

This theorem enables us to obtain stability results of the type

$$\sigma(A_n) < 1,$$

A_n again denoting an amplification matrix. A_n always depends on the step length τ_n. If $\tau_n = \tau$, τ constant, $A_n = A$, A constant. This result then implies that A^n tends to the zero-matrix as $n \to \infty$.

WACHSPRESS [18] also gives a corollary to theorem 5.2: Let $C = \prod_{i=1}^{\sim} C_i$, $C_i = I + \rho_i M_i^{-1} B$. If $M_i^T + M_i + \rho_i B$ is positive definite, then $\sigma(C) < 1$ for all $\rho_i > 0$. Hence, when assuming a finite set of non-constant stepsizes τ_n, this corollary can be used to show that the spectral radius of the resulting amplification matrix is smaller than one. We shall confine ourselves to the application of theorem 5.2.

5.3 Stability theorems

In the present section we list stability theorems for the greater part of the splitting formulas previously discussed. All these theorems deal with unconditional stability. The reader should be aware of the fact that the results are stated for the splitting formulas. To interpret a result for a splitting method based on a certain splitting formula, the type of splitting, as well as the underlying class of partial differential equations, has to be taken into consideration (see section 5.2).

5.3.1 Theorems for factorized stability functions

THEOREM 5.3.

1°. *The stability function of the formulas* (3.2),(4.2) *reads*

$$R(Z_1,Z_2) = (I-\tfrac{1}{2}Z_2)^{-1}(I-\tfrac{1}{2}Z_1)^{-1}(I+\tfrac{1}{2}Z_1)(I+\tfrac{1}{2}Z_2). \tag{5.8}$$

2°. *Let conditions* (5.6) *be satisfied and let* k = 2, *then* $\|R(\tau_n J_1,\tau_n J_2\|_2 < 1$ *for all* $\tau_n > 0$.

3°. *Let* $\tau_n = \tau$, τ *constant. If* $J_i+J_i^T$, i = 1,2, *is non-positive definite,* $R^n(\tau J_1,\tau J_2)$ *is uniformly bounded in* n *for all* $\tau > 0$.

PROOF. The derivation of the stability function (5.8) is straightforward. Part 2° is easily proved by making use of the commutativity and by applying part e) of theorem 5.1. To prove the last result we rewrite $R(\tau J_1,\tau J_2)$ as

$$R(\tau J_1,\tau J_2) = (I-\tfrac{1}{2}\tau J_2)^{-1}\tilde{R}(\tau J_1,\tau J_2)(I-\tfrac{1}{2}\tau J_2),$$

with

$$\tilde{R}(\tau J_1,\tau J_2) = (I-\tfrac{1}{2}\tau J_1)^{-1}(I+\tfrac{1}{2}\tau J_1)(I-\tfrac{1}{2}\tau J_2)^{-1}(I+\tfrac{1}{2}\tau J_2).$$

From part c) of theorem (5.1) it follows that

$$\|\tilde{R}(\tau J_1,\tau J_2)\|_2 \leq 1.$$

The uniform boundedness of $R^n(\tau J_1,\tau J_2)$ is now obtained from the relation

$$R^n(\tau J_1,\tau J_2) = (I-\tfrac{1}{2}\tau J_2)^{-1}\tilde{R}^n(\tau J_1,\tau J_2)(I-\tfrac{1}{2}\tau J_2)$$

and part b) of theorem 5.1. □

Function (5.8) is the stability function of the underlying splitting formulas for the implicit alternating direction methods of Peaceman-Rachford and Douglas-Rachford, discussed in section 3.1.1. As these methods are based on a differential operator splitting, part 2^o of the preceding theorem shows unconditional stability of the methods for the 2-dimensional version of equation (5.7). Further, part 3^o of the theorem shows that under less restrictive conditions than (5.6), a somewhat weaker form of unconditional stability is preserved.

The hopscotch methods, discussed in sections 3.1.2, 3.1.3, are based on the same splitting formula as the method of Peaceman-Rachford. It is beyond the scope of this paper to interpret the results of theorem (5.3) for hopscotch splittings. A nice stability result has been given by GOURLAY [7].

THEOREM 5.4.

1^o. *The stability function of the splitting formula for the alternating direction - locally one-dimensional method* (3.18) *is*

$$(5.9)\qquad R(Z_1,Z_2,Z_3) = (I-\tfrac{1}{2}Z_1)^{-1}(I+\tfrac{1}{2}Z_2)(I-\tfrac{1}{2}Z_3)^{-1}$$
$$(I+\tfrac{1}{2}Z_3)(I-\tfrac{1}{2}Z_2)^{-1}(I+\tfrac{1}{2}Z_1).$$

2^o. *Assume that conditions* (5.6) *with* k = 3 *hold, then* $\|R(\tau_n J_1,\tau_n J_2,\tau_n J_3)\|_2 < 1$ *for all* $\tau_n > 0$.

PROOF. Part 1^o follows from a trivial calculation. Part 2^o is proved by making use of the commutativity and by applying part e) of theorem 5.1. □

Applying this theorem to the integration of the 3-dimensional version of equation (3.7) by formula (3.18) with differential operator splitting reveals the unconditional stability of the integration process.

THEOREM 5.5.

1^o. *The stability function of the splitting formula for the locally one-dimensional method* (3.19) *is*

$$(5.10) \qquad R(Z_1,\ldots,Z_k) = \prod_{i=k}^{1} (I-\alpha Z_i)^{-1}(I+(1-\alpha)Z_i).$$

2^o. *Let* $\alpha = \frac{1}{2}$ *or* $\alpha = 1$. *Assume the matrices* $J_i+J_i^T$ *to be non-positive definite, then* $\|R(\tau_n J_1,\ldots,\tau_n J_k)\|_2 \leq 1$ *for all* $\tau_n > 0$.

3^o. *Let* $\alpha = \frac{1}{2}$ *or* $\alpha = 1$. *Assume the matrices* $J_i+J_i^T$ *to be negative definite, then* $\|R(\tau_n J_1,\ldots,\tau_n J_k)\|_2 < 1$ *for all* $\tau_n > 0$.

PROOF. Part 1^o follows again from a trivial calculation. Result 2^o and 3^o are immediate consequences of theorem 5.1. □

We see that the locally one-dimensional method is stable under less restrictive conditions than those of (5.6). For example, no commutativity is required.

5.3.2 Theorems for non-factorized stability functions

THEOREM 5.6.

1^o. *The stability function of the splitting formula for the method of approximation corrections* (3.20) *is*

$$(5.11) \qquad R(Z_1,\ldots,Z_k) = I + Z \prod_{i=k}^{1} (I-\tfrac{1}{2}Z_i)^{-1}.$$

2^o. *If conditions* (5.6) *are assumed, we have* $\sigma(R(\tau_n J_1,\ldots,\tau_n J_k)) < 1$ *for all* $\tau_n > 0$.

PROOF. The proof of part 1^o is again trivial. To prove the second part we apply theorem 5.2. Let $A_n = R(\tau_n J_1,\ldots,\tau_n J_k)$ and

$$M = \prod_{i=1}^{k} (I-\tfrac{1}{2}\tau_n J_i),$$

then $A_n = I + \tau_n JM^{-1}$. Because of the commutativity, A_n may be written as $A_n = I + \tau_n M^{-1}J$, and

$$M^T + M + \tau_n J = 2 \prod_{i=1}^{k} (I+\tfrac{1}{2}\tau_n \bar{J}_i) - \tau_n \sum_{i=1}^{k} \bar{J}_i,$$

where $\bar{J}_i = -J_i$ is symmetric and positive definite. This expression may be rewritten as

$$M^T + M + \tau_n J = 2I + P,$$

P being a sum of products of symmetric positive definite, commuting matrices. As a product of such matrices is also positive definite, 2I + P is positive definite, which proves part 2^o of the thorem. □

THEOREM 5.7.

1^o. *The stability function of the splitting formula for the method of stabilizing corrections* (3.21) *is*

$$(5.12) \qquad R(Z_1,\ldots,Z_k) = I + \prod_{i=k}^{1} (I-Z_i)^{-1}Z.$$

2^o. *If conditions* (5.6) *are assumed, we have* $\sigma(R(\tau_n J_1,\ldots,\tau_n J_k)) < 1$ *for all* $\tau_n > 0$.

PROOF. When applied to equations (5.4)-(5.5), the intermediate values $y_{n+1}^{(i)}$, i = 2(1)k, of formula (3.21) satisfy

$$(5.13) \qquad y_{n+1}^{(i)} = (I-\tau_n J_i)^{-1}[y_{n+1}^{(i-1)} - \tau_n J_i y_n].$$

By induction on i we now prove that

$$(5.14) \qquad y_{n+1}^{(i)} = \prod_{j=i}^{1} (I-\tau_n J_j)^{-1}[\prod_{j=1}^{i} (I-\tau_n J_j) + \tau_n J]y_n, \quad i = 2(1)k.$$

From (5.13) it follows that

$$y_{n+1}^{(i+1)} = (I-\tau_n J_{i+1})^{-1}[y_{n+1}^{(i)} - \tau_n J_{i+1} y_n]$$

By assuming that (5.14) is valid, we obtain

$$y_{n+1}^{(i+1)} = (I-\tau_n J_{i+1})^{-1} *$$

$$[\prod_{j=i}^{1}(I-\tau_n J_j)^{-1}\{\prod_{j=1}^{i}(I-\tau_n J_j) + \tau_n J\} - \tau_n J_{i+1}]y_n =$$

$$= (I-\tau_n J_{i+1})^{-1} *$$

$$[\prod_{j=i}^{1}(I-\tau_n J_j)^{-1}\{\prod_{j=1}^{i}(I-\tau_n J_j) + \tau_n J - \prod_{j=1}^{i}(I-\tau_n J_j)\tau_n J_{i+1}\}]y_n =$$

$$= \prod_{j=i+1}^{1}(I-\tau_n J_j)^{-1}[\prod_{j=1}^{i+1}(I-\tau_n J) + \tau_n J]y_n.$$

For i = 2 relation (5.14) follows from an easy calculation, which completes the induction. Further, by substituting i = k into (5.14) and writing

$$y_{n+1}^{(k)} = [I + \prod_{j=k}^{1}(I-\tau_n J_j)^{-1}\tau_n J]y_n,$$

the proof of part 1^o is completed. The proof of part 2^o is analogous to that of part 2^o of theorem 5.6. This is easy to see after inspection of both exressions for R. □

THEOREM 5.8.

1^o. *The stability function of the splitting formula for the method of stability corrections* (3.22) *is*

$$(5.15) \qquad R(Z_1,\ldots,Z_k) = I + \prod_{i=k}^{1}(I-\tfrac{1}{2}Z_i)^{-1}Z.$$

2^o. *If properties* (5.6) *are assumed, we have* $\sigma(R(\tau_n J_1,\ldots,\tau_n J_k)) < 1$ *for all* $\tau_n > 0$.

PROOF. The proof of part 1^o is analogous to that of the preceding theorem. For the proof of part 2^o we refer to theorem 5.6. □

When the formulas (3.20)-(3.22) are applied to equation (5.7) with a differential operator splitting of the right hand side, the theorems of this section show unconditional stability of the integration processes. Note that the stability function (5.15) for k = 2 is precisely function (5.8). Further, note that in case of commuting arguments function (5.15) equals function (5.11).

6. NUMERICAL EXAMPLES

The purpose of this section is to show the behaviour of ADI-type splitting methods when we change from problems with linearly coupled space derivatives to equations with non-linearly coupled derivatives. In order to draw conclusions from the numerical results we also give the results delivered by a line hopscotch method which can directly be applied to linear as well as to fully non-linear problems.

6.1 Methods used

In our numerical experiments we concentrated on the *non-linear* Peaceman-Rachford and Douglas-Rachford formulas which arise from (4.2') by choosing $(\alpha,\lambda) = (\frac{1}{2},\frac{1}{2})$ and $(\alpha,\lambda) = (0,1)$, respectively. It is easily verified that when applied to equations with linearly coupled space derivatives, the resulting splitting formulas belong to class (3.2'). The splitting function F was defined by (4.4) with

$$D = \tfrac{1}{2}I.$$

Together with these two ADI-type methods we applied the line hopscotch method generated by (3.2') and (3.15) with $\lambda = \beta = \gamma = \frac{1}{2}$.

In all experiments the Jacobian matrices used to solve the implicit equations were numerically evaluated by means of differences of right hand side evaluations and updated (if necessary) at the beginning of each Newton iteration process. Most of the examples were chosen in such a way that the implicit equations, to be solved at the first and second stage of the integration formulas, are linear, so that one Newton iteration suffices. The advantage is that we are not bothered by iteration strategies. But, to see the behaviour of the methods when several iterations are involved, we included one example where non-linear implicit equations are to be solved. The iteration process was stopped when two iterates differed less than

$$10^{-8}(1 + |U|)$$

in each gridpoint. When this criterion was not satisfied within 10 iterations the integration process was broken off (in the tables indicated by

∞). As predictor formula to start the Newton iteration we chose an extrapolation formula which guarantees second order accuracy after one iteration (cf. [20]).

In order to compare the computational effort of the various methods we have listed the average number of evaluations of the splitting function F(t,u,v) per integration step. In the tables this number is denoted by the letter E.

In the line hopscotch method the "implicit direction" was alternated after each integration step being horizontally implicit in all even-indexed steps and vertically implicit otherwise. (This implies that the computational effort involved to calculate Jacobian matrices is half that needed in the ADI type methods.)

In the tables given below we listed for each method, in addition to the number E, the *accuracy* obtained in terms of the number of correct digits, i.e. the number

$$A = -{}^{10}\log \mid \textit{maximum (relative error in the end point)} \mid .$$

When we draw conclusions from the (A,E)-values produced by the various methods, we have to bear in mind that the computational effort involved to compute Jacobian matrices, to perform LU-decompositions, etc, is not taken into account. This part of the integration process, however, is strongly related to error and stepsize control, and is completely left out of consideration in this paper. Thus, the tables in the next sections only evaluate the (iteration and) accuracy performance of the methods.

6.2 Linearly coupled space derivatives

Our first example is given by the equation

$$(6.1)\qquad \frac{\partial U}{\partial t} = U^{2m}\left[\frac{\partial^2 U}{\partial x_1^2} + \frac{\partial^2 U}{\partial x_2^2} - 2t(\sin(10\pi t) + x_1)\right] +$$

$$+ t(x_1^2+x_2)\left(\frac{\sin(10\pi t)}{t} + 10\pi\cos t\right) + x_1 x_2^2,\quad 0 \le t \le 1,\ (x_1,x_2)\in\Omega,$$

where m = 0 and Ω is given by the L-shaped region

$$(6.2)\qquad \Omega = \{(x_1,x_2)\,|\,(0<x_1<1,\ 0<x_2\le\tfrac{3}{7})\ \cup\ (0<x_1<\tfrac{4}{7},\ \tfrac{3}{7}\le x_2<1)\}.$$

Initial and Dirichlet-boundary conditions are prescribed and are chosen in such a way that (6.3) is the exact solution of the initial-boundary value problem:

$$(6.3)\qquad U(t,x_1,x_2) = t[(x_1^2+x_2)\sin(10\pi t) + x_1x_2^2].$$

The problem is converted into a system of 24 ordinary differential equations by replacing Ω with a grid Γ of square meshes with sides 1/7, by semi-discretizing (6.1) on this grid using standard symmetrical differences, and by substituting the boundary conditions where boundary values of U occur in the difference formulas. Note that the exact solution of this system is still given by (6.3) when (x_1,x_2) is restricted to the grid points of Γ.

In table 6.1 results are presented for equation (6.1) with m = 0.

Table 6.1 (A,E)-values for problem (6.1) with m = 0 and mesh side 1/7

Splitting method	$\tau_n = .02$	$\tau_n = .01$	$\tau_n = .005$
Peaceman-Rachford	(-.58,2)	(.03,2)	(.63,2)
Douglas-Rachford	(-.56,3)	(.04,3)	(.65,3)
Line hopscotch	(-.44,2)	(.31,2)	(.98,2)

These results show that the ADI-methods have a similar accuracy behaviour, the Peaceman-Rachford method being cheaper; the line hopscotch method is considerably more accurate in this case.

Our second example is again given by the equation (6.1) but now with m = 1 which makes the problem non-linear although the space derivatives are still linearly coupled in the right hand side. The results given in table 6.2 reveal that this non-linear case the ADI-methods are both reliable and more efficient than the line hopscotch method. Again the Peaceman-Rachford method is preferred to the Douglas-Rachford method.

Table 6.2 (A,E)-values for problem (6.1) with m = 1 and mesh side 1/7

Splitting method	$\tau_n = .02$	$\tau_n = .01$	$\tau_n = .005$
Peaceman-Rachford	∞	(.81,8.5)	(1.41,6.8)
Douglas-Rachford	∞	(.72,9.6)	(1.30,7.8)
Line hopscotch	∞	∞	(1.04,5.0)

6.3 Non-linearly coupled space derivatives

We now consider examples where the space derivatives are non-linearly coupled. Firstly, we solved

$$\frac{\partial U}{\partial t} = \frac{1}{1+t}\left[\frac{\partial^2 U}{\partial x_1^2} + \frac{\partial^2 U}{\partial x_2^2}\right] + \omega \frac{\partial U}{\partial x_1}\frac{\partial U}{\partial x_2} + \frac{x_2^2 - x_1^2 + 4\omega x_1 x_2}{(1+t)^2}, \tag{6.4}$$

$$0 \le t \le 1, \ (x_1, x_2) \in \Omega,$$

with $\omega = 1$ and Ω given by (6.2). Initial and Dirichlet-boundary conditions are determined by choosing (6.5) as the exact solution of the initial-boundary value problem:

$$U(t, x_1, x_2) = 1 + \frac{x_1^2 - x_2^2}{1+t}. \tag{6.5}$$

In the same way as done for the preceding examples this problem is converted into an initial value problem for a system of 24 ordinary differential equations by choosing the mesh sides equal to 1/7.

In table 6.3 the results are presented showing a similar behaviour for the ADI-methods as in the preceding examples: the Peaceman-Rachford method is more accurate and requires less computational effort than the Douglas-Rachford method. The line-hopscotch method is competitive for small integration steps but less efficient for larger step sizes.

Table 6.3 (A,E)-values for problem (6.4) with $\omega = 1$ and mesh size 1/7

Splitting method	$\tau_n = .1$	$\tau_n = .02$	$\tau_n = .01$
Peaceman-Rachford	(2.07,2)	(3.49,2)	(4.10,2)
Douglas-Rachford	(1.74,3)	(3.19,3)	(3.79,3)
Line hopscotch	(1.52,2)	(3.51,2)	(4.01,2)

Let us increase the non-linearity of the coupling of the space derivatives by choosing $\omega = 5$ in equation (6.4). The same methods now produce the results listed in table 6.4. The difference in performance of the three methods, already observable in the case $\omega = 1$, is more pronounced and shows that the Peaceman-Rachford method is the superior one in this example.

Table 6.4 (A,E)-values for problem (6.4) with $\omega = 5$ and mesh size 1/7

Splitting method	$\tau_n = .1$	$\tau_n = .02$	$\tau_n = .01$
Peaceman-Rachford	(1.93,2)	(3.37,2)	(3.97,2)
Douglas-Rachford	(1.72,3)	(3.17,3)	(3.78,3)
Line hopscotch	(1.37,2)	(3.54,2)	(4.00,2)

7. CONCLUDING REMARKS

As already observed in the introduction, each splitting method discussed in this paper consists of two components, viz. the splitting functions and the splitting formula. To some extent these two components are independent of each other. The splitting functions largely depend on the class of problems under consideration, so that we are not completely free in choosing them. Once a splitting has been found, which is appropriate to the problem to be solved, usually more than one splitting formula can be chosen to obtain a computationally attractive process. Since the order of consistency and the stability function of the splitting formulas do not

depend on the splitting functions, a suited splitting formula can be selected on the ground of accuracy and stability considerations.

In the paper the emphasis has been on the presentation and formulation of existing splitting methods. There is an abundant literature on this subject. For ease of survey we confined the discussion to the most important methods. Sections 4 and 6 has been added to illustrate the applicability of implicit alternating direction methods to non-linear problems with an arbitrary coupling between space derivatives. It should be noted that the numerical results of these methods, given in section 6, are still very tentative.

ACKNOWLEDGEMENTS. The authors would like to thank Mrs. M. Louter-Nool and Mr. B.P. Sommeijer who programmed the experiments. We also thank Mr. B.P. Sommeijer for his critical remarks during the investigations.

REFERENCES

[1] BUTCHER, J.C., *Implicit Runge-Kutta processes*, Math. Comp. 18, 50-64. 1964.

[2] DOUGLAS, J. Jnr., *On the numerical integration of* $u_{xx} + u_{yy} = u_t$ *by implicit methods*, J. Soc. Ind. Appl. MAth. 3, 42-65, 1955.

[3] DOUGLAS, J. Jnr. & H.H. RACHFORD Jnr., *On the numerical solution of heat conduction problems in two and three space variables*, Trans. Amer. Math. Soc. 82, 421-439, 1956.

[4] DOUGLAS, J. Jnr., *Alternating direction methods for three space variables*, Num. Math. 4, 41-63, 1962.

[5] DOUGLAS, J. Jnr. & J.E. GUNN, *A general formulation of alternating direction methods, Part I. Parabolic and hyperbolic problems*, Num. Math. 6, 428-453, 1964.

[6] DOUGLAS, J. Jnr. & T. DUPONT, *Galerkin methods for parabolic equations*, SIAM J. Numer. Anal. 7, 575-626, 1970.

[7] GOURLAY, A.R., *Hopscotch, a fast second order partial differential equation solver*, J. Inst. Math. Applics. 6, 375-390, 1970.

[8] GOURLAY, A.R. & G. Mc GUIRE, J. Inst. Math. Applics. 7, 216-227, 1971.

[9] GOURLAY, A.R. & A.R. MITCHELL, *On the structure of alternating direction implicit (A.D.I.) and locally one dimensional (L.O.D.) difference methods*, J. Inst. Math. Applics. 9, 80-90, 1972.

[10] GOURLAY, A.R., *Splitting methods for time-dependent partial differential equations*, in the proceedings of the 1976 conference: *The state of the art in numerical analysis*, ed. D.A.H. Jacobs, Academic Press, 1977.

[11] HENRICI, P., *Discrete variable methods in ordinary differential equations*, John Wiley & Sons, New York, 1962.

[12] KELLOG, R.B., *An alternating direction method for operator equations*, J. Soc. Ind. Appl. Math. 12, 848-854, 1964.

[13] PEACEMAN, D.W. & H.H. RACHFORD Jnr., *The numerical solution of parabolic and elliptic differential equations*, J. Soc. Ind. Appl. Math. 3, 28-41, 1955.

[14] RICHTMYER, R.D. & K.W. MORTON, *Difference methods for initial value problems*, Interscience, New York, 1967.

[15] STETTER, H.J., *Analysis of discretization methods for ordinary differential equations*, Springer-Verlag, Berlin, 1973.

[16] VAN DER HOUWEN, P.J. & J.G. VERWER, *A general formulation of linear splitting methods for ordinary and partial differential equations*, Report NW 44/77, Mathematisch Centrum, Amsterdam, 1977.

[17] VAN DER HOUWEN, P.J. & J.G. VERWER, *Non-linear splitting methods for semi-discretized parabolic differential equations*, Report NW 51/77, Mathematisch Centrum, Amsterdam, 1977.

[18] WACHSPRESS, E.L., *Stability of numerical solution of semi-discrete parabolic equations*, Comp. & Math. with Appls. 3, 131-133, 1977.

[19] YANENKO, N.N., *The method of fractional steps*, Springer-Verlag, Berlin, 1971.

[20] SOMMEIJER, B.P., *An* ALGOL 68 *implementation of two splitting methods for semi-discretized parabolic differential equations*, Note NN 15/77, Mathematisch Centrum, Amsterdam, 1977.