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One-Step Splitting Methods for Semi-Discrete Parabolic Equations

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Abstract — Zusammenfassung

One-Step Splitting Methods for Semi-Discrete Parabolic Equations. 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 autonomous semi-discrete equations

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

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.

Einschritt Split-Methoden für semi-diskrete parabolische Gleichungen. In dem Artikel werden speziell die Split-Methoden für parabolische Gleichungen mittels der Linienmethode besprochen. Bei diesen Methoden behandeln wir zuerst die Formulierung für autonome semi-diskrete Gleichungen

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

wobei f eine lineare Split-Relation $f(y)=\sum_{i=1}^{k} f_i(y)$ erfüllt. Eine Klasse von Einschritt-Integrationsformeln wird hier definiert welche alle bekannten Split-Methoden enthält, unter der Bedingung, daß die Funktionen f_i geschickt gewählt sind. Für eine Reihe von Methoden werden Stabilitätsergebnisse angegeben. Ferner wird das alternierende Richtungsverfahren für Probleme mit einer willkürlichen nicht-linearen Verbindung zwischen Raumableitungen diskutiert.

Keywords and phrases: Numerical analysis, ordinary differential equations, partial differential equations, method of lines, splitting methods.

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

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[17], 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 [14] to obtain an approximate solution of the original differential equation. If the discretization 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 exists 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* will be discussed.

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, 16], the locally one-dimensional methods [26], and the hopscotch methods [9, 10]. In the literature these methods are usually formulated and analyzed as direct grid methods. Examples of *explicit* splitting methods, designed for hyperbolic partial differential equations, can be found in [20, 8]. Such methods are related to explicit Runge-Kutta methods for ordinary differential equations.

We consider the numerical integration of the initial value problem for ordinary differential equations

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

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

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

We assume that (1.1) is obtained from semi-discretization of parabolic initial boundary value problems defined by t-independent differential operators. 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 functions 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 splitting 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 formula, 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 splitting (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. 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 [15], and a theorem given by Wachspress [25].

This paper is based on two institute reports [22, 23]. For the preparation of these reports the book of Yanenko [26] and the survey of Gourlay [12] were very useful.

2. Linear Splitting Formulas

Consider the m-stage, one-step integration formula

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

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 λ_{jli} 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 often occur. Observe that for $k = 1$, i.e. when no splitting is performed, scheme (2.1) reduces to an m-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

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

holds, where $y(t)$ denotes a sufficiently differentiable solution of 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 [22].

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. [14] or [19]).

Table 2.1. *Consistency conditions for (2.1)*

$p=1$	$\sum_{l=0}^{m} \lambda_{ml i}=1,\ i=1\,(1)\,k,$
$p=2$	$\sum_{l=1}^{m}\sum_{r=0}^{l} \lambda_{ml i}\lambda_{lr j}=\frac{1}{2},\ i,j=1\,(1)\,k,$
$p=3$	$\sum_{r=0}^{l} \lambda_{lr 1}=\sum_{r=0}^{l} \lambda_{lr 2}=\ldots=\sum_{r=0}^{l} \lambda_{lr k},\ l=1\,(1)\,m,$
	$\sum_{l=1}^{m} \lambda_{ml i}\left(\sum_{r=0}^{l} \lambda_{lr j}\right)^2=\frac{1}{3},\ i,j=1\,(1)\,k,$
	$\sum_{l=1}^{m}\sum_{r=1}^{l}\sum_{s=0}^{r} \lambda_{ml i}\lambda_{lr j}\lambda_{rs t}=\frac{1}{6},\ i,j,t=1\,(1)\,k.$

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 is noted that the discretization 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-stage formula

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

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 generates several known splitting methods. We will show this in the following subsections by specifying 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 $\partial\Omega$ denote the boundary curve of Ω, and consider a parabolic equation of the non-linear type

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

defined in the product set $\Omega \times (0, T]$. Further, assume the boundary conditions on $\partial\Omega \times (0, T]$ of the form

$$a(x_1, x_2)\, u + b(x_1, x_2)\, u_n = c(x_1, x_2),\ u_n \text{ normal derivative}. \tag{3.3'}$$

Superimpose a rectangular 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

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

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

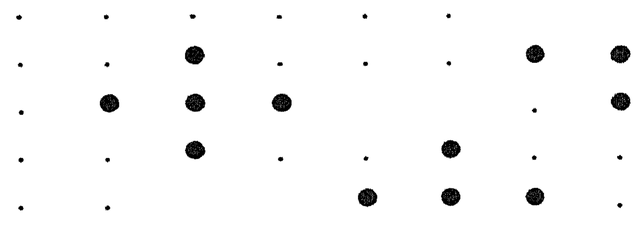

Fig. 3.1. A set of internal grid points

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

$$f(y) = f_1(y) + f_2(y) \tag{3.5}$$

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 and Rachford [16]:

$$y_{n+1}^{(1)} = y_n + \tfrac{1}{2}\tau_n [f_1(y_{n+1}^{(1)}) + f_2(y_n)],$$
$$y_{n+1} = y_{n+1}^{(1)} + \tfrac{1}{2}\tau_n [f_1(y_{n+1}^{(1)}) + f_2(y_{n+1})]. \tag{3.6}$$

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

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

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

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

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 $f_{\circ}$, $f_{\bullet}$, f_{+} and $f_{\times}$, such that

$$f(y) = f_{\circ}(y) + f_{\bullet}(y) + f_{+}(y) + f_{\times}(y), \tag{3.10}$$

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

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

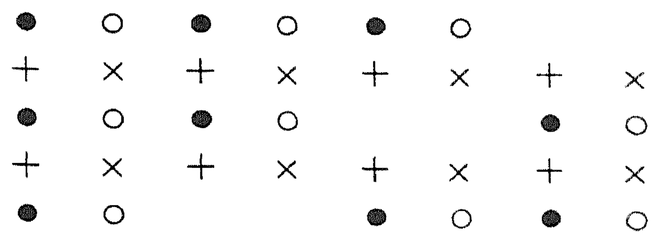

Fig. 3.2. Four subsets of gridpoints

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

$$f_1(y)=f_{\circ}(y)+f_{+}(y),$$
$$f_2(y)=f_{\circ}(y)+f_{\times}(y). \tag{3.12}$$

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 $\in \Omega_{\bullet} \cup \Omega_{\times}$, and then at the points $\in \Omega_{\circ} \cup \Omega_{+}$, 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. An additional advantage of hopscotch-type methods is that the explicit evaluations can be saved by rewriting them in the so-called fast form (see [9]).

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:

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

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

$$u_t=G(x_1, x_2, u, u_{x_1}, u_{x_2}, u_{x_1 x_1}, u_{x_1 x_2}, u_{x_2 x_2}), \tag{3.14}$$

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

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

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 $\in \Omega_{+} \cup \Omega_{\times}$, and then at the points $\in \Omega_{\circ} \cup \Omega_{\bullet}$, 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 functions (3.15) define the splitting along horizontal grid lines. In a similar way the splitting may be defined for vertical lines. 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. Test results of the line hopscotch method, written in its fast form and applied to non-autonomous equations, can be found in [13, 21].

3.2 Multi-Term Splitting Methods

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

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

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

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

where each f_i denotes the semi-discrete operator G_i, i.e. we use 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

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

It is easily verified that (3.18) is *second order* consistent. This type of splitting method has been suggested by Gourlay and Mitchell [11]. 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-stage formula

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

where α is still a free parameter. For every α the method is *first order* consistent. This type of splitting method emanates from Yanenko [26]. 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 usually equals $\frac{1}{2}$ or 1.

3.2.3 The Method of Approximation Corrections of Yanenko

Consider the $k+1$-stage formula

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

This type of splitting method also emanates from Yanenko [26], 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-stage formula

$$\begin{aligned} y_{n+1}^{(1)} &= y_n + \tau_n [f(y_n) - f_1(y_n) + f_1(y_{n+1}^{(1)})], \\ y_{n+1}^{(j)} &= y_{n+1}^{(j-1)} + \tau_n [f_j(y_{n+1}^{(j)}) - f_j(y_n)],\ j=2\,(1)\,k, \\ y_{n+1} &= y_{n+1}^{(k)}. \end{aligned} \tag{3.21}$$

For $k \leq 3$ this splitting method was introduced by Douglas and Rachford [3] and later, in its general form, formulated by Douglas and Gunn [5] (see also Yanenko [26]). 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-stage formula

$$\begin{aligned} y_{n+1}^{(1)} &= y_n + \tau_n [f(y_n) - \tfrac{1}{2} f_1(y_n) + \tfrac{1}{2} f_1(y_{n+1}^{(1)})], \\ y_{n+1}^{(j)} &= y_{n+1}^{(j-1)} + \tfrac{1}{2}\tau_n [f_j(y_{n+1}^{(j)}) - f_j(y_n)],\ j=2\,(1)\,k, \\ y_{n+1} &= y_{n+1}^{(k)}. \end{aligned} \tag{3.22}$$

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

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

Formula (4.2) is a one-step formula of the form (2.2) to which the usual definitions of consistency and convergence apply. A straightforward 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

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

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) lead to the linear Peaceman-Rachford and Douglas-Rachford methods.

Next, let $f(y)$ originate from (3.9), i.e. f does not satisfy a linear differential operator splitting. Using the notation of section (3.1.2), we define the function $F(v, w)$ by

$$\begin{aligned} F(v, w) = {} & f_{\circ}(D v_{\circ} + v_{\bullet} + w_{\times} + (I - D) w_{\circ}) + \\ & f_{\times}(D v_{\times} + v_{+} + w_{\circ} + (I - D) w_{\times}) + \\ & f_{\bullet}(D v_{\bullet} + v_{\circ} + w_{+} + (I - D) w_{\bullet}) + \\ & f_{+}(D v_{+} + v_{\times} + w_{\bullet} + (I - D) w_{+}), \end{aligned} \tag{4.4}$$

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 $\Omega_{\circ} \cup \Omega_{\bullet}$ and $\Omega_{+} \cup \Omega_{\times}$, 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 method with $\lambda = \frac{1}{2}$, i.e.

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

will be called the *non-linear Peaceman-Rachford method*, and the method with $\lambda = 1$, i.e.

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

the *non-linear Douglas-Rachford 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 were $u_t = u_{x_1 x_1} + u_{x_2 x_2}$. In other cases, however, e.g. for $u_t = u_{x_1 x_1} + \alpha u_{x_2 x_2}$, $\alpha \neq 1$, 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

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

For a definition of the splitting function $F(y, y, y)$ in this case, we refer to [23]. □

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 analysis [17]. 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 [15] and a theorem given in Wachspress [25].

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

$$R^{[0]}(Z_1, \ldots, Z_k) = I, \ I \text{ the unit matrix},$$

$$R^{[j]}(Z_1, \ldots, Z_k) = I + \sum_{l=0}^{j} \sum_{i=1}^{k} \lambda_{jli} Z_i R^{[l]}(Z_1, \ldots, Z_k), \ j = 1(1)m, \tag{5.3}$$

$$R(Z_1, \ldots, Z_k) = R^{[m]}(Z_1, \ldots, Z_k).$$

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

$$\frac{dy}{dt} = J y, \tag{5.4}$$

where

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

In fact, it is usually 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]:

$$\begin{aligned} &1^\circ. \text{ The matrices } J_i \text{ are symmetric and negative definite.} \\ &2^\circ. \text{ The matrices } J_i \text{ commute.} \end{aligned} \tag{5.6}$$

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 usually 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 [15] 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 [25], 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 [25] also gives a corollary to theorem 5.2: Let r be some positive integer, and let

$$C=\prod_{i=1}^{r} C_i,\ C_i=I+\rho_i M_i^{-1} B.$$

If $M_i^T+M_i+\rho_i B$ is positive definite for $i=1(1)r$, 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

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

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° of the preceding theorem shows unconditional stability of the methods for the 2-dimensional version of equation (5.7). Further, part 3° 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 [9].

Theorem 5.4:

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

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

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

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

Theorem 5.5:

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

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

2°, *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°. *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° follows again from a trivial calculation. Result 2° and 3° 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°. *The stability function of the splitting formula for the method of approximation corrections* (3.20) *is*

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

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

Proof: The proof of part 1° 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 $A_n = I + \tau_n J M^{-1}$. 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 re-written 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° of the theorem. □

Theorem 5.7:

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

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

2°. *If conditions* (5.6) *are assumed, we have* $\sigma\left(R(\tau_n J_1, \ldots, \tau_n J_k)\right) < 1$ *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

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

By induction on i we now prove that

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

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

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

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

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

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

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

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

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

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

Theorem 5.8:

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

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

2°. *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° is analogous to that of the preceding theorem. For the proof of part 2° 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. 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 functions 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. Section 4 has been added to illustrate the applicability of implicit alternating direction methods to non-linear problems with an arbitrary coupling between space derivatives.

We restricted our considerations to equations without t-dependent terms. This enables us to give a general presentation and formulation of splitting methods. Formally the various methods can be easily generalized for equations with t-dependent terms. However, when doing this, one should take into account that the t-dependent terms coming from time dependent boundary conditions will usually cause a drop in accuracy (cf. Fairweather and Mitchell [7]).

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