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TWO-STEP SPLITTING METHODS FOR SEMI-DISCRETE SECOND ORDER HYPERBOLIC PARTIAL DIFFERENTIAL EQUATIONS

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Two-step splitting methods for semi-discrete second order hyperbolic partial differential equations

by

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ABSTRACT

In this report splitting methods are discussed for a certain class of second order hyperbolic partial differential equations via the method of lines, and in particular the time integration will be discussed. A class of two-step integration formulas is defined, which contains several well-known splitting methods. The first-and second- order two-step splitting methods are unconditionally stable for a model problem. Numerical experiments are reported.

KEY WORDS & PHRASES : *Numerical analysis, ordinary differential equations, hyperbolic differential equations, method of lines, splitting methods*

1. INTRODUCTION

It is the purpose of this report to discuss splitting methods for second order hyperbolic partial differential equations (PDEs) via the *method of lines*. In the literature second order hyperbolic PDEs have been treated with alternating direction methods [2], locally one-dimensional methods [15] and hopscotch methods [5] formulated via the *direct grid approach*.

Let

$$(1.1) \qquad \frac{d^2y}{dt^2} = f(t,y), \qquad f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$$

denote a semi-discrete second order hyperbolic PDE, where we assume that f can be linearly split into k terms, k > 1 i.e.,

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

The functions f_i are called splitting functions [9] and depend on the original PDE and the type of semi-discretization.

In section 2 of this report, we define a general class of two-step integration formulas for the systems (1.1)-(1.2), which we shall call splitting formulas. We distinguish between *splitting functions* and *splitting formalas*, and a combination of both will be called a *splitting method* [9]. In section 3 a survey of known, linear splitting formulas is given.

In section 4 we introduce the multi-argument splitting

$$(1.3) \qquad F(t,y,\ldots,y) = f(t,y), \qquad F : \mathbb{R} \times \mathbb{R}^N \times \ldots \times \mathbb{R}^N \to \mathbb{R} \times \mathbb{R}^N ,$$

where the (nonlinear) splitting function F has m ($m \geq 2$) vector arguments [8,9]. For the systems (1.1)-(1.3) we define in this section a rather general class of two-step integration formulas.

The stability properties for the integration formula under consideration will be investigated for the *model problem* (the k-dimensional wave equation)

$$(1.4) \qquad \frac{\partial^2 y}{\partial t^2} = \sum_{i=1}^{k} \frac{\partial^2 y}{\partial x_i^2}, \quad 0 \le x_i \le 1 \quad , i = 1, \ldots, k$$

with zero-Dirichlet-boundary conditions. When we semi-discretize (1.4) using standard finite differences on an uniform grid, we obtain a linear system of ordinary differential equations (ODEs) of the form

$$(1.5) \qquad \frac{d^2 y}{dt^2} = Jy \quad , \quad J = \sum_{i=1}^{k} J_i$$

where J_i corresponds with $\partial^2/\partial x_i^2$. The matrices J and J_i have a *negative* eigenvalue spectrum and satisfy the common eigensystem condition [2,8].

In section 5 a few splitting functions are summarized, which are frequently used in practice. Finally, in section 6 some splitting methods are illustrated with numerical examples.

In this report we consider first and second order splitting methods which are unconditionally stable for the model problem (1.4). This limitation is a consequence of Dahlquist's theorem: a linear multistep method that is A-stable cannot have order greater than two [1] .

2. LINEAR SPLITTING FORMULAS

Consider the m-stage, 2 - step integration formula

$$y_{n+1}^{(j)} = \mu^{(j)} y_n + (1-\mu^{(j)}) y_{n-1} + \tau^2 \sum_{i=1}^{k} b_2^{(ji)} f_i(t_{n-1}+\gamma_{ji}\tau, y_{n-1}) +$$

$$+ \tau^2 \sum_{i=1}^{k} b_1^{(ji)} f_i(t_{n-1}+\beta_{ji}\tau, y_n) + \tau^2 \sum_{\ell=1}^{j} \sum_{i=1}^{k} \lambda_{j\ell i} f_i(t_{n-1}+\alpha_{j\ell i}\tau, y_{n+1}^{(\ell)}),$$

$$j = 1\ (1)\ m,$$

$$y_{n+1} = y_{n+1}^{(m)} \quad , \quad \mu^{(m)} = 2,$$

where y_{n-1}, y_n denote the numerical approximations respectively at $t = t_{n-1}$, $t = t_n$ and $\tau \equiv t_{n+1} - t_n = t_n - t_{n-1}$. Each formula from class (2.1) is called a *linear 2-step splitting formula*. The parameters $b_1^{(ji)}$, $b_2^{(ji)}$, $\mu^{(j)}$, $\alpha_{j\ell i}$, β_{ji}, γ_{ji} and $\lambda_{j\ell i}$ serve to make this scheme a consistent and stable approximation to (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 future reference, we consider two linear 2-step methods for the second-order ODE (1.1). The first-order consistent linear 2-step method

$$(2.2)\qquad y_{n+1} = 2y_n - y_{n-1} + \tau^2 f(t_{n+1}, y_{n+1})$$

and the second-order consistent linear 2-step method

$$(2.3)\qquad y_{n+1} = 2y_n - y_{n-1} + \frac{\tau^2}{4}[f(t_{n-1},y_{n-1}) + 2f(t_n,y_n) + f(t_{n+1},y_{n+1})]$$

belong to the class (2.1). The formula (2.3) has the smallest error constant among second order accurate linear multistep methods [1,8]. Both methods generate several splitting formulas and therefore the formulas (2.2) and (2.3) will be called *generating formulas*.

2.1. Consistency conditions

Expanding y_{n+1} in a Taylor series at the point (t_{n-1}, y_{n-1}) the order conditions for scheme (2.1) can be derived. Conditions up to order $p = 2$ are listed in Table 2.1. The derivation of these conditions is straightforward.

Table 2.1 Consistency conditions for (2.1)

$p = 1$	$b_1^{(mi)} + b_2^{(mi)} + \sum_{\ell=1}^{m} \lambda_{m\ell i} = 1$	, $i = 1(1)k$,
$p = 2$	$b_1^{(mi)} + \sum_{\ell=1}^{m} \mu^{(\ell)} \lambda_{m\ell i} = 1$	, $i = 1(1)k$,
	$b_2^{(mi)} \gamma_{mi} + b_1^{(mi)} \beta_{mi} + \sum_{\ell=1}^{m} \alpha_{m\ell i} \lambda_{m\ell i} = 1$	, $i = 1(1)k$.

By deleting the last condition in table 2.1 the order conditions for scheme (2.1) are also listed in table 2.1 for an autonomous system (i.e., $\frac{d^2y}{dt^2} = f(y)$). For an autonomous system the integration formula (2.1) is third order consistent when, in addition to the order conditions up to to order p = 2,

$$(2.4)\qquad b_1^{(mi)} + \sum_{\ell=1}^{m} (\mu^{(\ell)})^2 \lambda_{m\ell i} = 1/6 \quad , \ i = 1(1)k,$$

$$(2.5)\qquad b_1^{(mi)} + 2\sum_{\ell=1}^{m} \lambda_{m\ell i} [\frac{\mu^{(\ell)}}{2} + b_1^{(\ell j)} + b_2^{(\ell j)}] + $$

$$+ 2\sum_{\ell=1}^{m} \sum_{r=1}^{\ell} \lambda_{m\ell i} \lambda_{\ell rj} = 7/6, \ i,j = 1(1)k.$$

For convergence of a p-th order consistent scheme (2.1) we refer to convergence results of linear multistep methods (cf.[7,12]).

2.2. Stability

DOUGLAS AND GUNN [2] give a general formulation and stability analysis of ADI methods for second order hyperbolic PDEs via the *direct grid approach*.

By using the *method of lines* the characteristic equation of the integration formula (2.1) can be obtained in a direct manner (cf.[8]) and is for m > 1 defined by the formal relations

$$(1- \sum_{i=1}^{k} \lambda_{mmi} z_i) \zeta^2 - (2+ \sum_{i=1}^{k} b_1^{(mi)} z_i) \zeta + (1- \sum_{i=1}^{k} b_2^{(mi)} z_i)$$

$$- \sum_{\ell=1}^{m-1} \sum_{i=1}^{k} \lambda_{m\ell i} z_i R^{(\ell)}(\zeta) = 0,$$

$$R^{(1)}(\zeta) = (1- \sum_{i=1}^{k} \lambda_{11i} z_i)^{-1} \{(\mu^{(1)} + \sum_{i=1}^{k} b_1^{(1i)} z_i) \zeta +$$

$$(2.6a)\qquad + 1- \mu^{(1)} + \sum_{i=1}^{k} b_2^{(1i)} z_i\},$$

$$R^{(\ell)}(\zeta) = (1 - \sum_{i=1}^{k} \lambda_{\ell\ell i}\, z_i)^{-1}\{(\mu^{(\ell)} + \sum_{i=1}^{k} b_1^{(\ell i)} z_i)\, \zeta +$$

$$+ 1 - \mu^{(\ell)} + \sum_{i=1}^{k} b_2^{(\ell i)} z_i$$

$$+ \sum_{q=1}^{\ell-1} \sum_{i=1}^{k} \lambda_{\ell q i}\, z_i\, R^{(q)}(\zeta)\} \ , \ \ell = 2(1)\, m-1 ,$$

where z_i and z represent eigenvalues of $\tau^2 J_i$ and $\tau^2 J$, respectively. For $m=1$ the characteristic equation of (2.1) is defined by

$$\text{(2.6b)} \qquad \zeta^2 - R^{(1)}(\zeta) = 0.$$

In order to have an *infinite negative* interval of stability for formulas of type (2.1), the characteristic equations (2.6a) and (2.6b) should have their roots on or within the unit circle for all *negative* z and z_i.

We conclude this section with the formulas for the characteristic equation of the linear 2-step methods (2.2) and (2.3). The characteristic equation of the first order formula (2.2) given by

$$\text{(2.7)} \qquad (1-z)\, \zeta^2 - 2\, \zeta + 1 = 0$$

has its roots *within* the unit circle for all negative z, whereas the characteristic equation of the second order formula (2.3) given by

$$\text{(2.8)} \qquad (1-\frac{z}{4})\, \zeta^2 - (2 + \frac{z}{2})\, \zeta + 1 - \frac{z}{4} = 0$$

has its roots *on* the unit circle [8]. A simple calculation reveals that the roots of (2.7) satisfy the relation

$$|\ \zeta_j(z)\ | = \frac{\sqrt{1+|z|}}{\sqrt{1-z}} \simeq \frac{1}{\sqrt{|z|}} \ , \ j = 1,2, \text{ as } |z| \to \infty ,$$

i.e. formula (2.2) has a very strong damping effect on the higher harmonics.

3. A SURVEY OF LINEAR SPLITTING FORMULAS

In this section we consider only splitting formulas of type (2.1); for the definition of useful splitting functions we refer to section 5. Several examples of known unconditionally stable splitting methods are discussed in the following subsections.

The splitting formulas will be considered for a rather general class of nonlinear initial-boundary value problems given by

$$\text{(3.1a)} \qquad \frac{\partial^2 u}{\partial t^2} = \sum_{i=1}^{k} G_i(t,x,u,\frac{\partial^2 u}{\partial x_i^2}) \;, \quad x = (x_1,\dots,x_k) \;, \qquad x \in \Omega \cup \delta\,\Omega \,,$$

$$\text{(3.1b)} \qquad u(t_0,x) = u_0(x) \;, \quad \frac{\partial u}{\partial t}(t_0,x) = v_0(x) \;, \qquad x \in \Omega \cup \delta\,\Omega \,,$$

$$\text{(3.1c)} \qquad a_0(t,x)\,u(t,x) + a_1(t,x)u_n = a_2(t,x),\ u_n \text{ normal derivative}, \qquad x \in \delta\,\Omega,$$

where Ω is a bounded and path-connected region in the $(x_1,\dots,x_k)$-space with sides parallel to the coordinate axes and $\delta\Omega$ is the boundary curve of Ω. By applying the method of lines, that is by replacing the region $\Omega \cup \delta\,\Omega$ by a rectangular grid with grid lines parallel to the coordinate axes the equation (3.1a) and the boundary condition (3.1c) together convert into a system of ODEs (1.1).

The splitting formulas in the subsections 3.1 and 3.2 are suitable for the k-dimensional problem (3.1a) - (3.1c), whereas in the other subsections only splitting formulas for 2-dimensional problems, i.e. k=2 in (3.1a) - (3.1c), are considered.

The splitting formulas together with a suitable splitting function could also be applied to the more general 2-dimensional nonlinear initial-boundary value problems

$$\text{(3.2a)} \qquad \frac{\partial^2 u}{\partial t^2} = G(t,x_1,x_2,u,u_{x_1x_1},u_{x_2x_2}), \qquad (x_1,x_2) \in \Omega \cup \delta\,\Omega$$

and

$$\text{(3.2b)} \qquad \frac{\partial^2 u}{\partial t^2} = G(t,x_1,x_2,u,u_{x_1x_1},u_{x_1x_2},u_{x_2x_2}), \qquad (x_1,x_2) \in \Omega \cup \delta\Omega ,$$

with the boundary and initial conditions defined in a similar way as for problem (3.1a). However, for the problems (3.2a) and (3.2b) numerical results obtained by splitting methods are hardly available in the literature.

3.1. The fractional step methods of Konovalov

Consider the k-stage formula

$$\text{(3.3)} \qquad \begin{aligned} y_{n+1}^{(1)} &= 2y_n - y_{n-1} + \tau^2 f_1(t_{n+1},y_{n+1}^{(1)}) , \\ y_{n+1}^{(j)} &= y_{n+1}^{(j-1)} + \tau^2 f_j(t_{n+1},y_{n+1}^{(j)}) , \quad j = 2(1)k. \end{aligned}$$

This splitting formula was introduced by Konovalov [10] and is *first order* consistent. For this formula the characteristic equation is given by

$$\text{(3.4)} \qquad \prod_{j=1}^{k} (1-z_j)\, \zeta^2 - 2\zeta + 1 = 0.$$

From Hurwitz's criterion (cf.[12,p.81]) it follows that the roots of (3.4) are *within* the unit circle for all negative z_j.

In the same article Konovalov suggested another k-stage formula

$$\text{(3.5)} \qquad \begin{aligned} y_{n+1}^{(1)} &= 2y_n - y_{n-1} + \tau^2 f_1(t_{n+1},y_{n+1}^{(1)}) + \tau^2 \sum_{i=2}^{k} f_i(t_{n+1},y_n) , \\ y_{n+1}^{(j)} &= y_{n+1}^{(j-1)} + \tau^2 f_j(t_{n+1},y_{n+1}^{(j)}) - \tau^2 f_j(t_{n+1},y_n) , \quad j = 2(1)k \end{aligned}$$

with the characteristic equation

$$\text{(3.6)} \qquad \prod_{j=1}^{k} (1-z_j)\, \zeta^2 - [\prod_{j=1}^{k} (1-z_j) + z+1]\, \zeta + 1 = 0 .$$

It is easily verified that (3.5) is again *first order* consistent and that the roots of (3.6) are *within* the unit circle. The splitting formulas (3.3) and (3.5) have (2.2) as the generating formula. The splitting formulas of Konovalov are also applicable to 2-dimensional hyperbolic PDEs containing a mixed derivative [10] and hyperbolic PDEs arising in the theory of elasticity for plane problems [11].

3.2. A second order 2-step splitting formula

Consider the k-stage splitting formula

$$
(3.7)\qquad
\begin{aligned}
y_{n+1}^{(1)} &= 2y_n - y_{n-1} + \frac{\tau^2}{4}\,[f(t_{n-1},y_{n-1}) + 2f(t_n,y_n) + f_1(t_{n+1},y_{n+1}^{(1)})],\\
y_{n+1}^{(j)} &= y_{n+1}^{(j-1)} + \frac{\tau^2}{4}\, f_j(t_{n+1},y_{n+1}^{(j)}) \qquad , \ j = 2(1)k.
\end{aligned}
$$

For this *second order* consistent formula the characteristic equation is given by

$$
(3.8)\qquad \prod_{i=1}^{k} (1-\tfrac{1}{4}z_j)\,\zeta^2 - (2+\tfrac{z}{2})\,\zeta + 1 - \tfrac{z}{4} = 0.
$$

For negative z and z_j - values (3.8) has its roots *within* the unit circle, whereas the characteristic equation (2.8) of the generating formula (2.3) has its roots *on* the unit circle. As far as we know, the formula (3.7) has not been discussed in the literature. When we compare the number of function evaluations of the formulas (3.3) and (3.7) per integration step, it is clear that (3.7) requires one extra function evaluation.

A *second order* analogue of (3.5) is the k-stage stabilizing corrections splitting formula (cf.[2,8])

$$
(3.9)\qquad
\begin{aligned}
y_{n+1}^{(1)} &= 2y_n - y_{n-1} + \frac{\tau^2}{4}\,[f(t_{n-1},y_{n-1}) + 2\,f(t_n,y_n) + f_1(t_{n+1},y_{n+1}^{(1)}) + \\
&\qquad\qquad + \sum_{i=2}^{k} f_i(t_n,y_n)]\ ,\\
y_{n+1}^{(j)} &= y_{n+1}^{(j-1)} + \frac{\tau^2}{4}\,[f_j(t_{n+1},y_{n+1}^{(j)}) - f_j(t_n,y_n)]\ , \quad j = 2(1)k
\end{aligned}
$$

with the characteristic equation

$$
(3.10)\qquad \prod_{j=1}^{k}(1-\tfrac{1}{4}z_j)\,\zeta^2 - [\prod_{j=1}^{k}(1-\tfrac{1}{4}z_j) + \tfrac{3}{4}z + 1]\,\zeta + 1 - \tfrac{z}{4} = 0.
$$

It is easily verified that (3.10) has its roots *within* the unit circle.

3.3. The method of approximating factorization

Consider the 2-stage formula

$$(3.11)\qquad \begin{aligned} y_{n+1}^{(1)} &= y_n + \frac{\tau^2}{2} f_1(t_n, y_{n+1}^{(1)}) , \\ y_{n+1} &= 2y_{n+1}^{(1)} - y_{n-1} + \frac{\tau^2}{2} [f_2(t_{n-1}, y_{n-1}) + f_2(t_{n+1}, y_{n+1})] . \end{aligned}$$

This *second order* consistent splitting formula has been suggested by D'YAKONOV [3] for the 2-dimensional wave equation (see also YANENKO [17,p.50]). The characteristic equation of the method of approximating factorization (3.11) is given by

$$(3.12)\qquad (1 - \tfrac{1}{2} z_2)(1 - \tfrac{1}{2} z_1)\zeta^2 - 2\zeta + (1 - \tfrac{1}{2} z_2)(1 - \tfrac{1}{2} z_1) = 0 .$$

The roots of (3.12) lie *on* the boundary of the unit circle.

3.4. A method of Lees

Consider the 2-stage formula

$$(3.13)\qquad \begin{aligned} y_{n+1}^{(1)} &= 2y_n - y_{n-1} + \eta\tau^2 f_1(t_{n-1}, y_{n-1}) + (1-2\eta)\tau^2 f_1(t_n, y_n) \\ &\quad + \tau^2 f_2(t_n, y_n) + \eta\tau^2 f_1(t_{n+1}, y_{n+1}^{(1)}) , \\ y_{n+1} &= y_{n+1}^{(1)} + \eta\tau^2 [f_2(t_{n-1}, y_{n-1}) - 2 f_2(t_n, y_n) + f_2(t_{n+1}, y_{n+1})] , \end{aligned}$$

where η is still a free parameter. This splitting formula was introduced by LEES [13] (see also MITCHELL [14]). It is easily verified that (3.13) is *second order* consistent for every choice of η. The choice $\eta = 1/12$ leads for an autonomous system even to a third order consistent splitting formula, which can be easily verified by using (2.4) and (2.5).

The characteristic equation is given by

$$(3.14)\qquad (1-\eta z_2)(1-\eta z_1)\zeta^2 - \zeta\,[2 + z(1-2\eta) + 2\eta^2 z_1 z_2] + (1-\eta z_2)(1-\eta z_1) = 0.$$

Application of Hurwitz's criterion reveals that (3.14) has its roots *on* the unit circle for all negative z_1 and z_2 if $\eta \geq 1/4$.

3.5. The locally one-dimensional method of Samarskii

Consider the 3-stage formula

$$(3.15)\qquad \begin{aligned} y_{n+1}^{(1)} &= \tfrac{1}{2}(y_{n-1}+y_n) - \frac{\tau^2}{8}[f_2(t_{n-1},y_{n-1}) + f_2(t_n,y_n)], \\ y_{n+1}^{(2)} &= 2y_n - y_{n+1}^{(1)} + \frac{\tau^2}{4}[f_1(t_n,y_{n+1}^{(1)}) + f_1(t_n,y_{n+1}^{(2)})], \\ y_{n+1} &= 2y_{n+1}^{(2)} - y_n + \frac{\tau^2}{4}[f_2(t_n,y_n) + f_2(t_{n+1},y_{n+1})]. \end{aligned}$$

This splitting formula was introduced by SAMARSKII [15] (see also MITCHELL [14])for the 2-dimensional wave equation. The locally one-dimensional splitting formula (3.15) is *second order* consistent and its characteristic equation is given by

$$(3.16)\qquad (1-\tfrac{1}{4}z_1)(1-\tfrac{1}{4}z_2)\zeta^2 - (2+\tfrac{z}{2})\,\zeta + 1 - \tfrac{z}{4} = 0.$$

From Hurwitz's criterion it follows that the roots of (3.16) are *within* the unit circle.

4. NON-LINEAR SPLITTING FORMULAS

In this section some non-linear splitting formulas are discussed for general nonlinear systems (1.1), where the vector function f satisfies the non-linear splitting relation (1.3). Such general nonlinear systems are for example obtained from the semi-discretization of the initial-boundary value problems (3.1a -3.1c),(3.2a) and (3.2b). For the definition of useful splitting functions we refer to section 5.

4.1. The method of successive corrections

Consider the splitting (1.3) with only 2 vector arguments, i.e.

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

Let the splitting function $F(t,u,v)$ have "simply structured" Jacobian matrices $J_1 = \partial F/\partial u$ and $J_2 = \partial F/\partial v$. Then a class of 2-step splitting formulas belonging to the more general class defined in [8] reads

$$
\begin{aligned}
&y_{n+1}^{(0)} = y_{n+1}^{(pred)}, \quad \Sigma_n = 2y_n - y_{n-1} + b_1\tau^2 f(t_n,y_n) + b_2\tau^2 f(t_{n-1},y_{n-1}),\\
&y_{n+1}^{(j)} = \Sigma_n + b_0\tau^2 F(t_{n+1},y_{n+1}^{(j)},y_{n+1}^{(j-1)}) \quad , \quad j = 1,3,5,\ldots \quad ,\\
&y_{n+1}^{(j)} = \Sigma_n + b_0\tau^2 F(t_{n+1},y_{n+1}^{(j-1)},y_{n+1}^{(j)}) \quad , \quad j = 2,4,6,\ldots \quad ,\\
&y_{n+1} = y_{n+1}^{(m)} \quad ,
\end{aligned}
\tag{4.2}
$$

where $y_{n+1}^{(pred)}$ is a predictor formula of order q. The integration formula defined by (4.2) is consistent of order $\min\{p,2m+q\}$, where p is the order of the generating formula $y_{n+1} = \Sigma_n + b_0\tau^2 f(t_{n+1},y_{n+1})$ (cf. [8]). Substitution of a particular splitting function into (4.2) leads to a scheme which will be called *the method of successive corrections*.

In the stability analysis we confine ourselves to the model problem (1.4) with $k = 2$, where the matrices $b_0\tau^2 J_1$ and $b_0\tau^2 J_2$ have a common eigensystem with negative eigenvalues z_1 and z_2, respectively. In [8] the characteristic equation of the method of successive corrections is given, where Σ_n corresponds to a linear k-step formula and $y_{n+1}^{(pred)}$ corresponds to an one-step formula or an explicit linear $\hat{k}$-step formula. The behaviour of the roots $\zeta(z_1,z_2)$ of the characteristic equation for large values of $|z_1|$ and $|z_2|$ is important. As $|\zeta|$ is smaller for $|z_1|$, $|z_2| \gg 1$, the stronger is the damping of the higher harmonics in the numerical error. We can only have asymptotic stability of (4.2) for even m values if the predictor formula is also asymptotically stable. Therefore the formulas

(4.3a) $$y^{(pred)}_{n+1} = y_n \quad \text{with } q = -1$$
and
(4.3b) $$y^{(pred)}_{n+1} = 2y_n - y_{n-1} \quad \text{with } q = 0$$

seem to be plausible choices.

Choosing in (4.2) m even,

$$y^{(pred)}_{n+1} = y_n, b_0 = b_2 = 1/4 \text{ and } b_1 = 1/2$$

we obtain a *second-order* splitting formula with the characteristic equation

(4.4) $$(1-z)\zeta^2 - \{2(1+z) - \tilde{R}(1+3z)\}\zeta + (1-\tilde{R})(1-z) = 0,$$

where $\tilde{R} = \left[\frac{z_1 z_2}{(1-z_1)(1-z_2)}\right]^{m/2}$, $z = z_1 + z_2$. Observing that for m even

$$0 < \tilde{R} < 1 \quad ,$$

it is easily verified that the roots of (4.4) are *within* the unit circle, whereas the characteristic equation (2.8) of the generating formula (2.3) has its roots *on* the unit circle. In [8] the case m = 2 was considered. Replacing the predictor formula (4.3a) by (4.3b) leads also the a *second-order* splitting formula with the characteristic equation

(4.4)' $$(1-z)\zeta^2 - 2(1+z-2\tilde{R}z)\zeta + 1 - z = 0 .$$

However, the roots of (4.4)' lie *on* the boundary of the unit circle.

Choosing in (4.2) m even,

$$y^{(pred)}_{n+1} = y_n, b_1 = b_2 = 0 \text{ and } b_0 = 1$$

we obtain a *first-order* splitting formula with the characteristic equation

(4.5) $$(1-z)\zeta^2 - [2 - \tilde{R}(1+z)]\ \zeta + 1 - \tilde{R} = 0.$$

From Hurwitz's criterion it follows that (4.5) has its roots *within* the unit circle for all negative z_1 and z_2, just as the characteristic equation (2.7) of the generating formula (2.2). Replacing the predictor formula (4.3a) by (4.3b) leads also to a *first-order* splitting formula with the characteristic equation

$$(4.5)' \qquad (1-z)\,\zeta^2 - 2(1-\tilde{R}z)\,\zeta + 1 - \tilde{R}z = 0,$$

which has again its roots *within* the unit circle.

For $|z_1|$, $|z_2| \to \infty$ the first order approximations of the dominant root of (4.4) and (4.5) are of the form (cf.[8])

$$\zeta \cong 1 + 2\,m\left(\frac{1}{z_1} + \frac{1}{z_2}\right)$$

and

$$\zeta \cong 1 + \frac{m}{2}\left(\frac{1}{z_1} + \frac{1}{z_2}\right),$$

respectively. Hence, for a given even value of m and the predictor formula (4.3a) the second order splitting formula has a slightly stronger damping of the higher harmonics than the first order splitting formula.

Furthermore, comparing the number of function evaluations of both formulas per integration step (both with the same value of m) , it is clear that the second order splitting formula requires one extra function evaluation.

4.2. The method of stabilizing corrections

Let the splitting function $F\,(t,u_1,\ldots,u_m)$ satisfy condition (1.3), let $J_j = \partial F/\partial u_j$, $j = 1,2,\ldots,m$ have a simple band structure, and consider the m-stage splitting formula

$$y_{n+1}^{(0)} = y_{n+1}^{(pred)},\quad \Sigma_n = 2y_n - y_{n-1} + b_1\tau^2 f(t_n,y_n) + b_2\tau^2 f(t_{n-1},y_{n-1}),$$

$$y_{n+1}^{(1)} = \Sigma_n + \mu_1\tau^2 F\,(t_{n+1},y_{n+1}^{(1)},y_{n+1}^{(0)},\ldots,y_{n+1}^{(0)}) + (b_0-\mu_1)\tau^2 f(t_{n+1},y_{n+1}^{(0)}),$$

(4.6)

$$y_{n+1}^{(j)} = y_{n+1}^{(j-1)} + \mu_j\tau^2\,[\,F(t_{n+1},y_{n+1}^{(0)},\ldots,y_{n+1}^{(0)},y_{n+1}^{(j)},y_{n+1}^{(0)},\ldots,y_{n+1}^{(0)})$$

$$- f(t_{n+1},y_{n+1}^{(0)})\,],\quad j = 2,3,\ldots,m,$$

$$y_{n+1} = y_{n+1}^{(m)},$$

where $y_{n+1}^{(pred)}$ is a predictor formula of order q and $y_{n+1}^{(j)}$ occurs at the j-th place in the row of vector arguments of F. A straightforward Taylor expansion reveals that formula (4.6) with the predictor formula (4.3a) is consistent of first order when

$$b_0 + b_1 + b_2 = 1 , \tag{4.7}$$

second order consistent when, in addition,

$$b_1 + 2b_0 = 1 , \tag{4.8a}$$

$$b_0 + b_1 + \mu_j = 1 , \quad j = 1(1)m . \tag{4.8b}$$

The order conditions of (4.6) with the predictor formula (4.3b) are given by (4.7) and (4.8a). Substitution of a particular splitting function into (4.6) leads to a scheme which will be called the *method of stabilizing corrections* [2,8].

Choosing in (4.6)

$$y_{n+1}^{(pred)} = y_n, \; b_1 = b_2 = 0 \text{ and } b_0 = 1$$

we obtain a first-order consistent splitting formula. For the model problem (1.4) with k = m, the characteristic equation of this splitting formula assumes the form

$$\prod_{j=1}^{m} (1-\mu_j z_j)\zeta^2 - [\prod_{j=1}^{m}(1-\mu_j z_j) + z + 1]\zeta + 1 = 0, \tag{4.9}$$

where the z_j denote the eigenvalues of the matrices $\tau^2 J_j$. It can be proved that (4.9) has its roots *within* the unit circle for all negative z_j if $\mu_j \geq 1/2$, j = 1(1)m. For $\mu_j = 1$, j = 1(1)m and the differential operator splitting function (cf.[8,9])

$$F(t,u_1,u_2,\ldots,u_m) = \sum_{i=1}^{m} f_i (t,u_i) \tag{4.10}$$

we obtain the earlier mentioned splitting formula of Konovalov (3.5). Replacing (4.3a) by (4.3b) leads also to a *first order* splitting formula with the characteristic equation

$$(4.9)' \qquad \prod_{j=1}^{m} (1-\mu_j z_j)\zeta^2 - 2\,[z + \prod_{j=1}^{m} (1-\mu_j z_j)]\zeta + \prod_{j=1}^{m} (1-\mu_j z_j) + z = 0\,.$$

From Hurwitz's criterion it follows that (4.9)' has its roots *within* the unit circle for all negative z_j if $\mu_j \geq 3/4$, $j = 1(1)m$.

Choosing in (4.6)

$$y_{n+1}^{(pred)} = y_n\,,\ b_0 = b_2 = 1/4,\ b_1 = 1/2 \text{ and } \mu_j = 1/4 \text{ for } j = 1(1)m$$

we obtain a *second-order* consistent splitting formula with the characteristic equation

$$(4.11) \qquad \prod_{j=1}^{m} (1-\tfrac{1}{4} z_j)\,\zeta^2 - [\prod_{j=1}^{m} (1-\tfrac{1}{4} z_j) + \frac{3z}{4} + 1]\,\zeta + 1 - \frac{z}{4} = 0.$$

The roots of (4.11) are *within* the unit circle for all negative z_j.

Choosing in (4.6)

$$y_{n+1}^{(pred)} = 2y_n - y_{n-1}\,,\ b_0 = b_2 = 1/4 \text{ and } b_1 = 1/2$$

we obtain also a *second-order* splitting formula with the characteristic equation

$$(4.11)' \qquad \prod_{j=1}^{m} (1-\mu_j z_j)\zeta^2 - [2 \prod_{j=1}^{m} (1-\mu_j z_j) + z]\zeta + \prod_{j=1}^{m} (1-\mu_j z_j) = 0.$$

However, the roots of (4.11)' lie *on* the boundary of the unit circle for all negative z_j if $\mu_j \geq 1/4$, $j = 1(1)m$.

The method of stabilizing corrections requires one evaluation of Σ_n and (m+1)-evaluations of F, whereas the method of successive corrections requires one evaluation of Σ_n and m evaluations of F.

5. SPLITTING FUNCTIONS

In the preceding sections we only derived splitting formulas, which can be selected on the ground of accuracy, stability considerations and computational efficiency. Substitution of a particular splitting function into a splitting formula leads to a splitting method. In this section, we summarize briefly a few splitting functions, which depend on the class of problems under consideration. For a more complete discussion of these splitting functions we refer to [8,9] . Some suitable splitting functions for the splitting formulas discussed in this report are:

1°. The *differential operator splitting function* [8,9] for a (2k+1) - point coupled (nonlinear) function f in (1.1) which originates from the semi-discretization of a k-dimensional hyperbolic PDE (3.1).

2°. The *odd-even* and *line hopscotch splitting function* [8,9] for a 5-point coupled (nonlinear) function f in (1.1).

3°. The *alternating direction implicit splitting function* [9] for a 5-point coupled (nonlinear) function f in (1.1).

Functions f derived from the 2-dimensional hyperbolic initial-boundary value problems (3.1) with k = 2 and (3.2a) satisfy a 5-point coupling. To 9-point coupled systems (1.1) the line hopscotch splitting function can also be applied together with a particular splitting formula. Such systems arise by semi-discretizing hyperbolic equations containing a mixed derivative (see section 3).

The splitting formulas discussed in section 4 can be combined with each splitting function, whereas the splitting formulas in section 3 can be combined only with the differential operator splitting function and the hopscotch splitting functions.

6. NUMERICAL EXPERIMENTS

The purpose of this section is to show that the splitting formulas together with a suitable splitting function can be applied to nonlinear hyberbolic initial-boundary value problems. To some extent the components of each splitting method discussed in this report, viz. the splitting function and the splitting formula, are independent of each other [9]. For a linear problem we illustrate that a certain type of splitting function can be combined with more than one type of splitting formula.

6.1. The test examples

The initial-boundary value problems we tested are all of the form

$$(6.1)\qquad \frac{\partial^2 u}{\partial t^2} = \alpha(t,x_1,x_2,u)\left[\frac{\partial^2 u^r}{\partial x_1^2} + \frac{\partial^2 u^r}{\partial x_2^2}\right] + v(t,x_1,x_2)$$

defined on $\{(t,x_1,x_2)\mid 0 \le t \le 1, (x_1,x_2) \in \Omega\}$, where Ω is given by

$$\Omega = \{(x_1,x_2)\mid 0 \le x_1,x_2 \le 1\}.$$

A splitting of $v = \frac{1}{2}v + \frac{1}{2}v$ was used in all experiments. The initial and Dirichlet boundary conditions follow from the exact solution given in table 6.1. By using standard differences the problems were semi-discretized on a uniform grid Ω_h with mesh width h. Evidently the components of the right-hand side function f in (1.1) are coupled according to a five-point molecule.

Table 6.1. Specification of the test examples

Example	Solution	$\alpha(t,x_1,x_2,u)$	$v(t,x_1,x_2)$	r
I	$1+e^{-t}(x_1^2+x_2^2)$	1	$e^{-t}(x_1^2+x_2^2-4)$	1
II	$1+e^{-t}(x_1^2+x_2^2)$	$100\cos^2\left[(x_1+x_2)u\right]$	$e^{-t}\left\{x_1^2+x_2^2 - 400\cos^2\left[(x_1+x_2)(1+e^{-t}(x_1^2+x_2^2))\right]\right\}$	1
III	$\frac{1}{2}(x_1+x_2)\sin(2\pi t)$	$\frac{x_1+x_2}{2(1+t)}$	$-2\pi^2(x_1+x_2)\sin(2\pi t) - \frac{3(x_1+x_2)^2}{4(1+t)}\sin^3(2\pi t)$	3

6.2. Methods used.

Three splitting formulas were applied to the examples I - III (see table 6.1). In our experiments we used the first order consistent formula (3.3) with k = 2, the second order consistent formula (3.7) with k = 2 and the second order splitting version of the method of successive corrections defined by (4.2) with m even, $b_1 = \frac{1}{2}$, $b_0 = b_2 = \frac{1}{4}$, i.e.,

$$
(6.2)\quad
\begin{aligned}
&y_{n+1}^{(0)} = y_{n+1}^{(pred)}, \quad \sum_n = 2y_n - y_{n-1} + \frac{\tau^2}{2} f(t_n,y_n) + \frac{\tau^2}{4} f(t_{n-1},y_{n-1}),\\
&y_{n+1}^{(j)} = \sum_n + \frac{\tau^2}{4} F(t_{n+1},y_{n+1}^{(j)},y_{n+1}^{(j-1)}), \quad j = 1,3,5,\ldots,m-1,\\
&y_{n+1}^{(j)} = \sum_n + \frac{\tau^2}{4} F(t_{n+1},y_{n+1}^{(j-1)},y_{n+1}^{(j)}), \quad j = 2,4,6,\ldots,m,\\
&y_{n+1}^{(j)} = y_{n+1}^{(m)}, \quad m \text{ even}.
\end{aligned}
$$

In the experiments we tested the predictor formulas (4.3a) and (4.3b) and chose m = 2 and m = 4.

For all the examples the splitting formulas are combined with the differential operator splitting function (D.O.splitting). Note that in the differential operator splitting the inhomogeneous term $v(t,x_1,x_2)$ will be split into $\frac{1}{2}v + \frac{1}{2}v$. For the linear problem I the formulas (3.3) and (3.7) are also combined with the odd-even hopscotch splitting function (O-E H.splitting).

The tridiagonal Jacobian matrices, used to solve the implicit equations by means of a Newton-type process, were obtained by analytical differentiation. In case of constant partial derivatives $\partial f/\partial y$, these matrices were determined once; in all other cases they were updated every integration step at the points (t_n,y_n). In all experiments the implicit equations were solved with one Newton iteration. As initial approximation to start the Newton iteration in the first stage of the splitting methods we chose an extrapolation formula. In the scheme {(4.3a),(6.2)} we used formula (4.3a) as initial approximation and in the other schemes we used formula (4.3b) as initial approximation. In the other stages we used in the Newton-type process the solution of the preceding stage as predictor.

In order to compare the computational effort of the various methods we have listed in the tables of results the number of f-evaluations per integration step. The splitting formula (3.3) costs one complete f-evaluation per integration step. The splitting formulas (3.7) and (6.2) require the functions $f(t_n,y_n)$ and $f(t_{n-1},y_{n-1})$ in every integration step. For both formulas one function evaluation per integration step can be saved, when in the implementation $f(t_n,y_n)$ is stored in an array with N components, where N is equal to the number of interior grid points of Ω_h. Thus, the formulas (3.7) and (6.2) cost per integration step 2 and (m+1) f-evaluations, respectively. In our comparison of the computational effort of the various methods we have not taken into account the evaluation of the Jacobian matrices, the LU-decompositions, the solution of tridiagonal systems of linear equations, etc.

6.3. Numerical results

The two starting values were obtained from the exact solution of the initial-boundary value problems.

The accuracy is measured by the number of correct digits in the end point $t = 1$, i.e.

$$(6.3) \qquad sd = - {}^{10}\log \left| \text{maximum absolute error in } t = 1 \right| .$$

From (6.3) it follows (see also LAMBERT [12,p.257]) that on halving the integration step τ the value of sd should increase by $p\,{}^{10}\log 2 \cong .3p$ for a method of order p (and τ sufficiently small).

In the tables of results given below the values of the pair (f,sd) are listed where f denotes the number of f-evaluations per integration step.

Table 6.2a (f,sd)-values for example I obtained by (3.3) and (3.7) together with differential operator (D.O) splitting and odd-even hopscotch (O-E H.) splitting.

h	τ	(3.3) with D.O.splitting	(3.3) with O-E H.splitting	(3.7) with D.O.splitting	(3.7) with O-E H.splitting
1/10	1/5	(1,2.37)	(1,.72)	(2,2.94)	(2,1.47)
	1/10	(1,2.78)	(1,1.02)	(2,3.61)	(2,2.31)
	1/20	(1,3.0)	(1,1.63)	(2,4.18)	(2,3.12)
	1/40	(1,3.33)	(1,2.38)	(2,4.75)	(2,3.80)
1/20	1/5	(1,2.22)	(1,0.5)	(2,2.92)	(2,0.95)
	1/10	(1,2.77)	(1,0.62)	(2,3.53)	(2,1.4)
	1/20	(1,3.0)	(1,0.95)	(2,4.07)	(2,2.38)
	1/40	(1,3.33)	(1,1.61)	(2,4.62)	(2,3.16)

In table 6.2a is illustrated for the linear example I that the splitting methods lose accuracy when the boundary conditions are time-dependent and if $h \to 0$, which is a well-known phenomenon [4,16]. Table 6.2a shows that the asymptotic order of the formulas (3.3) and (3.7) with the D.O. splitting is more or less reached, whereas with the O-E H.splitting a higher order of accuracy is shown. The splitting formulas in combination with the odd-even hopscotch splitting functions are less accurate and more sensitive to grid refinement than with the differential operator splitting function. Notice that the splitting formulas with the D.O. splitting require the solution of tridiagonal systems of linear equations, whereas with the O-E H.splitting only scalar linear equations have to be solved. Therefore a comparison based on f-evaluations is far from complete. The splitting formulas with O-E H. splitting satisfy the situation where a quick solution with little effort and not too great accuracy is required.

Table 6.2b (f,sd)-values for example I obtained by {(4.3a),(6.2)} and {(4.3b),(6.2)} with the differential operator splitting function and m = 2,4.

		{(4.3a),(6.2)}		{(4.3b),(6.2)}	
h	τ	m = 2	m = 4	m = 2	m = 4
1/10	1/5	(3,1.98)	(5,2.09)	(3,2.66)	(5,2.81)
	1/10	(3,2.88)	(5,3.66)	(3,3.98)	(5,4.25)
	1/20	(3,3.74)	(5,4.98)	(3,4.83)	(5,4.97)
	1/40	(3,4.55)	(5,5.64)	(3,5.65)	(5,5.64)
1/20	1/5	(3,1.33)	(5,1.6)	(3,2.12)	(5,2.42)
	1/10	(3,2.21)	(5,3.23)	(3,3.0)	(5,3.73)
	1/20	(3,3.17)	(5,4.35)	(3,4.32)	(5,5.01)
	1/40	(3,4.07)	(5,5.67)	(3,5.56)	(5,5.67)

In table 6.2b results are listed for example I but now for the method of successive corrections (6.2) with differential operator splitting. For m = 2 the scheme {(4.3b), (6.2)} is considerably more accurate than {(4.3a),(6.2)}. For m = 4 and $\tau \geq 1/20$ a similar conclusion can be drawn. Both schemes are rather sensitive to grid refinement. Table 6.2b also illustrates the effect of the value of m on the accuracy. For this range of τ-values the asymptotic order p = 2 is not clearly shown. Only for m = 4 the scheme {(4.3b),(6.2)} has the tendency to show its asymptotic order.

Comparing the results in the tables 6.2a and 6.2b we observe that especially for large τ values the method of the successive corrections is more sensitive to grid refinement than (3.3) and (3.7) with D.O. splitting. In the higher accuracy range {(4.3b),(6.2)} with m = 2 is the most efficient in terms of the total number of f-evaluations. For lower accuracies the method (3.7) with D.O. splitting becomes the more efficient one.

Table 6.3. (f,sd)-values for example II with h = 1/10.
Each formula uses D.O. splitting.

Formula	τ= 1/20	τ= 1/40	τ= 1/80
(3.3)	(1,2.83)	(1,2.91)	(1,3.18)
(3.7)	(2,3.7)	(2,4.14)	(2,4.67)
{(4.3a),(6.2)}, m = 2	*	*	(3,3.39)
{(4.3a),(6.2)}, m = 4	*	(5,2.89)	(5,4.55)
{(4.3b),(6.2)}, m = 2	*	(3,3.32)	(3,5.23)
{(4.3b),(6.2)}, m = 4	*	(5,4.03)	(5,5.9)

In table 6.3 results are listed for the nonlinear example II obtained with various formulas together with D.O. splitting. Instability is indicated by an asterisk. For large τ-values (3.7) is superior to the method of successive corrections, whereas the method of successive corrections {(4.3b), (6.2)} with m = 2 is competitive for τ = 1/80. Again increasing m improves the accuracy in the method of successive corrections considerably. The results in table 6.3 show that only the asymptotic order of the formulas (3.3) and (3.7) is more or less reached. The best choice for the predictor formula in (6.2) is again (4.3b)

Table 6.4. (f,sd)-values for example III with h = 1/10
The splitting formulas are combined with the differential operator splitting function.

Formula	τ= 1/10	τ= 1/20	τ= 1/40
(3.3)	(1,-.07)	(1,.1)	(1,.31)
(3.7)	(2,.58)	(2,1.26)	(2,1.84)
{(4.3a),(6.2)} , m = 2	(3,.63)	(3,1.23)	(3,1.83)
{(4.3a),(6.2)} , m = 4	(5,.63)	(5,1.23)	(5,1.83)
{(4.3b),(6.2)} , m = 2	(3,.37)	(3,1.23)	(3,1.83)
{(4.3b),(6.2)} , m = 4	(5,.64)	(5,1.23)	(5,1.83)

In table 6.4 the results are presented for the nonlinear example III with $h = 1/10$ showing that for $\tau \geq 1/20$ the effect of the choice of the predictor formula and the value of m in the method of successive corrections on the accuracy is negligible. For this example (3.7) with D.O. splitting is the most efficient method. The results show the correct order behaviour of the second order methods. The first order method (3.3) has the tendency to show its asymptotic order.

From the results of the three problems the following conclusions can be drawn:

- Using (4.3b), i.e. $y_{n+1}^{(pred)} = 2y_n - y_{n-1}$, as predictor formula in the method of successive corrections (6.2) instead of (4.3a) ($y_{n+1}^{(pred)} = y_n$) is worthwhile.
- For large τ-values (3.7) with the differential operator splitting function is the most efficient method.
- For higher accuracies the scheme {(4.3b),(6.2)} with $m = 2$ and differential operator splitting is preferable in the examples I and II.

7. CONCLUDING REMARKS

In this report a survey is given of the most important splitting methods for second order hyperbolic PDEs via the method of lines. In the literature the linear splitting formulas discussed in section 3 together with the differential operator splitting function are usually formulated and analysed as direct grid methods for the multi-dimensional wave equation with Dirichlet boundary conditions.

Using the predictor formula (4.3a) the second order splitting formulas discussed in section 4 have a stronger damping of the higher harmonics than using the predictor formula (4.3b).

It is known that splitting methods will usually lose accuracy when the boundary conditions are time-dependent (cf. FAIRWEATHER and MITCHELL [4]). This phenomenon was investigated in [4,16] for a class of splitting methods for parabolic PDEs and in [6] for a class of splitting methods for second order hyperbolic PDEs. Following the approach of SOMMEIJER et al. [16] the boundary-value correction can also be derived for splitting methods for a rather general class of hyperbolic initial-boundary value problems defined by (3.1a)-(3.1b). These aspects will be subject for future research.

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