A NOTE ON B-STABILITY OF SPLITTING METHODS

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Abstract. An important requirement on numerical methods for the integration of nonlinear stiff initial value problems is B-stability. In many applications it is also convenient to use splitting methods to take advantage of the special structure of the differential operator that define the model. The purpose of this paper is to provide a necessary and sufficient condition for the B-stability of additive Runge-Kutta methods. We also present a family of B-stable fractional step Runge-Kutta methods.

1. Introducion

In the recent literature much interest has been devoted to numerical integration of nonlinear stiff problems defined by operators that may be decompose on a sum of two or more parts. Several physical phenomena are described by these problems. We mention, for instance, reactive flow processes and combustion theory [13], multi-pahse flow in heterogeneous porous media [9], chemical reaction problems, atmospheric circulation problems [11], air pollution [14], etc. To obtain accurate numerical solutions for these problems, it is desirable to use numerical methods with good stability properties and, in addition, that take into account the special structure of the equations.

We focus our atenttion in the numerical solution of nonlinear stiff systems of ODE's, that may be viewed as a semi-discrete version of a stiff PDE's. For the time integration of these problems, the concept of B-stability, introduced by J.C. Butcher [6] for standard Runge-Kutta schemes, turned out to be crucial in the analysis of the numerical methods. A commonly used approach to the solution of these problems is based on splitting methods [12]. In the last decades, the emergence of new methods for special problems, leads us to the class of additive methods, which contain, as particular case, the class of alternating direction and fractional step schemes [4]. This work is devoted to the

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study of the B-stability properties for the class of Additive Runge-Kutta methods.

The paper is organized as follows. We start, in the next section, by presenting the motivation for the definition of additive Runge-Kutta methods. Then, after that definition, we introduce, as a particular case, the subclass of fractional step Runge-Kutta methods. In Section 3 we present the concepts of B-stability and algebraic stability. The main result of this paper is the necessary and sufficient condition for the B-stability of additive Runge-Kutta methods. Also in this section, we introduce the notion of AN-stability for linear non-autonomous stiff problems and B-stability for nonlinear ones. Section 4 is devoted to fractional step Runge-Kutta methods. In this section we particularize the main result of this paper to this class of methods. A class of B-stable fractional step Runge-Kutta methods is also presented.

2. Additive Runge-Kutta methods

Let us consider an initial value problem

$$\left\{ \begin{array}{lcl} y' & = & f^{[1]}(t,y) + \cdots + f^{[N]}(t,y), \\ y(0) & = & y_0, \end{array} \right. \tag{2.1}$$

where $f^{[\nu]} : \mathbb{R}_0^+ \times \mathbb{R}^D \longrightarrow \mathbb{R}^D$, $\nu = 1, \ldots, N$, are vectorial functions with components $f^{[\nu]i}$, $i = 1, ..., D$.

If, in (2.1), $N = 2$ and $f^{[1]}$ is stiff while $f^{[2]}$ is not, then it is common to combine an implicit integrator for $f^{[1]}$ with an explicit integrator for $f^{[2]}$. For instance, in a reaction-diffusion partial differential problem we may combine an implicit method for the diffusion with an explicit one for the reaction [2].

In this paper, we are special interested in the case where each part $f^{[\nu]}$, $\nu = 1, ..., N$, is stiff. This situation occurs, for instance, in molecular dynamics applications where the different $f^{[\nu]}$ may correspond to forces of different stiffness. Is is sometimes inappropriate to sample the net force f; one may wish to sample the stiffer parts more frequently than the softer parts. This leads to the idea of multiple time-step methods [3]. An example, with $N = 2$, of a multiple time-step method is given by the time-symmetric concatenation

$$\psi^{\mathrm{MP}}_{h,\alpha f^{[1]}} \circ \psi^{\mathrm{MP}}_{h,(1-2\alpha) f^{[1]} + f^{[2]}} \circ \psi^{\mathrm{MP}}_{h,\alpha f^{[1]}}, \tag{2.2}$$

where α is a real constant and $\psi^{\mathrm{MP}}_{h,g}$ denotes a step of length h of the implicit midpoint rule applied to the differential system with right-hand side g. Clearly (2.2) is a multiple time-step method that uses $f^{[2]}$ less frequently than $f^{[1]}$.

To take into account the special structure of the right hand side of the equation, let us consider the class of Additive Runge-Kutta methods defined in the following way [7].

Definition 2.1. An Additive Runge-Kutta (ARK) method of s stages and N levels is a one-step numerical method which, for a known approximation y_n to $y(t_n)$, obtain the approximation y_{n+1} to $y(t_{n+1})$, with $t_{n+1} = t_n + h$, where h is called the step size, according to the process

$$\begin{cases} Y_{n,i} &= y_n + h\sum_{\nu=1}^{N}\sum_{j=1}^{s} a_{ij}^{[\nu]} f^{[\nu]}(t_n + c_j h, Y_{n,j}) \\ y_{n+1} &= y_n + h\sum_{\nu=1}^{N}\sum_{i=1}^{s} b_i^{[\nu]} f^{[\nu]}(t_n + c_i h, Y_{n,i}). \end{cases} \tag{2.3}$$

The coefficients of the method may be organized in the Butcher tableau

$$\begin{array}{c|c|c|c|c} \mathrm{c} & A^{[1]} & A^{[2]} & \cdots & A^{[N]} \\ \hline & b^{[1]T} & b^{[2]T} & \cdots & b^{[N]T} \end{array}, \tag{2.4}$$

where $c = [c_1, ..., c_s]^T$ and, for $\nu = 1, ..., N$, $b^{[\nu]} = [b_1^{[\nu]}, ..., b_s^{[\nu]}]^T$ and $A^{[\nu]} = \left(a_{ij}^{[\nu]}\right)_{i,j=1}^{s}$.

Note that the multiple time-step method (2.2) is also an ARK method (2.3), with $N = 2$. In fact, if the differential system (2.1) is autonomous, (2.2) is the ARK method with tableau

$$\begin{array}{|ccc|ccc} \frac{\alpha}{2} & 0 & 0 & 0 & 0 & 0 \\ \alpha & \frac{1-2\alpha}{2} & 0 & 0 & \frac{1}{2} & 0 \\ \alpha & 1-2\alpha & \frac{\alpha}{2} & 0 & 1 & 0 \\ \hline \alpha & 1-2\alpha & \alpha & 0 & 1 & 0 \end{array}. \tag{2.5}$$

An important subclass of the ARK methods is class of fractional step Runge-Kutta methods defined as follows [4].

Definition 2.2. A Fractional Step Runge-Kutta (FSRK) method is an ARK method (2.3) which verifies:

(1) $a_{ii}^{[\nu]} \geq 0$, for $i = 1, ..., s$, and $\nu = 1, ..., N$, and $a_{ij}^{[\nu]} = 0$, for all $j > i$;

(2) $\left|b_j^{[\nu]}\right| + \sum_{i=1}^{s}\left|a_{ij}^{[\nu]}\right| = 0 \Rightarrow \left|b_j^{[\mu]}\right| + \sum_{i=1}^{s}\left|a_{ij}^{[\mu]}\right| \neq 0$, for $\nu, \mu = 1, ..., N$ such that $\mu \neq \nu$, and $i, j = 1, ..., s$;

(3) $a_{ii}^{[\mu]} a_{ii}^{[\nu]} = 0$, for $\nu, \mu = 1, ..., N$ such that $\mu \neq \nu$, and $i = 1, ..., s$.

According to the property (2) of the previous definition, a FSRK method given by (2.3) can be expressed in a condensed way in the form

$$
\begin{array}{c|c}
 & \theta^T \\
\hline
\mathrm{c} & A \\
\hline
 & b^T
\end{array}\,, \tag{2.6}
$$

with the vector b given by

$$b = \left(b_j^{[\theta_j]}\right)_{j=1}^{s} = \sum_{\nu=1}^{N} b^{[\nu]},$$

the matrix A by

$$A = \left(a_{ij}^{[\theta_j]}\right)_{i,j=1}^{s} = \sum_{\nu=1}^{N} A^{[\nu]}$$

and $\theta = [\theta_1, ..., \theta_s]^T$ where $\theta_j \in \{1, ..., N\}$ satisfy

$$\sum_{\substack{\nu=1\\ \nu\neq\theta_j}}^{N} \left(\left|b_j^{[\nu]}\right| + \sum_{i=1}^{s} \left|a_{ij}^{[\nu]}\right|\right) = 0, \qquad \text{for } j = 1, ..., s.$$

With this notation, a FSRK method may be written in the form

$$
\left\{
\begin{array}{rcl}
Y_{n,i} & = & y_n + h\sum_{j=1}^{s} a_{ij}^{[\theta_j]} f^{[\theta_j]}(t_n + c_j h, Y_{n,j}) \\
y_{n+1} & = & y_n + h\sum_{i=1}^{s} b_i^{[\theta_i]} f^{[\theta_i]}(t_n + c_i h, Y_{n,i}).
\end{array}
\right. \tag{2.7}
$$

3. B-stable additive Runge-Kutta methods

It is well known that when solving stiff ODE's is important to consider A-stable methods. This stability property belong to the so-called linear stability theory. When we deal with non-linear problems this theory is lacking rigor. A more convenient stability concept is the notion of B-stability which theory is well known for standard Runge-Kutta methods [6], [5], [8]. We now generalize this notion to the class of ARK methods.

Definition 3.1. An ARK method (2.3) is called B-satble if, for $\nu = 1, ..., N$, the contractivity condition

$$< f^{[\nu]}(t, y) - f^{[\nu]}(t, z), y - z >\leq 0, \qquad t \geq 0, \qquad \forall y, z \in \mathbb{R}^D, \tag{3.1}$$

implies for all $h \leq 0$

$$\|y_{n+1} - \tilde{y}_{n+1}\| \leq \|y_n - \tilde{y}_n\|\,, \tag{3.2}$$

where y_n and $\tilde{y}_n$ and $\tilde{y}_{n+1}$ are the numerical solutions defined by the method from y_n and $\tilde{y}_n$, respectively.

Our goal is to find methods with the same contractivity property. To characterize stable methods, let us introduce the notion of algebraic stability for the class of ARK methods (2.3).

Definition 3.2. If an ARK method (2.3) is such that the matrices

(i) $B^{[\nu]} := \operatorname{diag}\left(b_1^{[\nu]}, \ldots, b_s^{[\nu]}\right)$, $\nu = 1, ..., N$, and

(ii) $M^{[\nu\mu]} := B^{[\nu]}A^{[\mu]} + A^{[\nu]T}B^{[\mu]} - b^{[\nu]}b^{[\mu]T}$, $\nu, \mu = 1, ..., N$,

are non-negative is said to be algebraically stable.

We may now state the following result that is a generalization of the corresponded one for the standard Runge-Kutta case [10].

Theorem 3.3. *A sufficient condition for an ARK method (2.3) to be B-stable is to be algebraically stable.*

Proof: Let us consider

$$v_0 = y_n - \tilde{y}_n, \quad v_i = Y_{n,i} - \tilde{Y}_{n,i}, \quad v = y_{n+1} - \tilde{y}_{n+1}$$

and

$$w_i^{[\nu]} = h\left[f^{[\nu]}(t_n + c_i h, Y_{n,i}) - f^{[\nu]}(t_n + c_i h, \tilde{Y}_{n,i})\right].$$

With this notation we have

$$\begin{aligned}\|v\|^2 &= \|v_0\|^2 + 2\sum_{\nu=1}^{N}\sum_{i=1}^{s} b_i^{[\nu]} < v_0, w_i^{[\nu]} > + \sum_{\nu,\mu=1}^{N}\sum_{i,j=1}^{s} b_i^{[\nu]} b_j^{[\mu]} < w_i^{[\nu]}, w_j^{[\mu]} > \\ &= \|v_0\|^2 + 2\sum_{\nu=1}^{N}\sum_{i=1}^{s} b_i^{[\nu]} < v_i, w_i^{[\nu]} > - \sum_{\nu,\mu=1}^{N}\sum_{i,j=1}^{s} m_{i,j}^{[\eta\mu]} < w_i^{[\nu]}, w_j^{[\mu]} > .\end{aligned}$$

If the matrices $B^{[\nu]}$ and $M^{[\nu\mu]}$, $\nu, \mu = 1, ..., N$, are non-negative, then $\|v\|^2 \leq \|v_0\|^2$, because, by hypothesis $< v_i, w_i^{[\nu]} > \leq 0$. $\square$

Before proving the converse result, we introduce the notion of AN-stability. In order to define this concept, let us consider the non-autonomous linear test problem

$$y' = \sum_{\nu=1}^{N} \lambda^{[\nu]}(t) y(t), \quad \lambda^{[\nu]}(t) \in \mathbb{C}, \quad t \geq 0, \qquad y(0) = y_0. \tag{3.3}$$

If we apply the ARK method (2.3) to this problem we obtain

$$\left\{\begin{aligned} Y_n &= e y_n + \sum_{\nu=1}^{N} A^{[\nu]}\xi^{[\nu]} Y_n \\ y_{n+1} &= y_n + \sum_{\nu=1}^{N} b^{[\nu]}\xi^{[\nu]} Y_n e. \end{aligned}\right. \tag{3.4}$$

where $Y_n = [Y_{n,1}, ..., Y_{n,s}]^T$, $e = [1, ..., 1]^T$ and, for $\nu = 1, ..., N$,

$$\xi^{[\nu]} = \text{diag}\left(\xi_1^{[\nu]}, ..., \xi_s^{[\nu]}\right), \tag{3.5}$$

with

$$\xi_i^{[\nu]} = h\lambda^{[\nu]}(t_n + c_i h), \qquad i = 1, ..., s.$$

If the matrix

$$\Xi = I - \sum_{\mu=1}^{N} A^{[\mu]}\xi^{[\mu]} \tag{3.6}$$

is regular the ARK method (3.4) may be written in the form

$$y_{n+1} = R(\xi)y_n,$$

with

$$R(\xi) := R(\xi^{[1]}, ..., \xi^{[N]}) = 1 + \sum_{\nu=1}^{N} b^{[\nu]T}\xi^{[\nu]}\Xi^{-1}e. \tag{3.7}$$

Definition 3.4. The ARK method (2.3) is called AN-stable if

$$|R(\xi)| \leq 1, \tag{3.8}$$

for all $\xi^{[\nu]}$ given by (3.5) with $\xi_i^{[\nu]} \neq \xi_i^{[\nu]}$ whenever $c_i \neq c_j$ and such that $\text{Re}(\xi_i^{[\nu]}) \leq 0$, for $i = 1, ..., s$.

Note that, according to this definition, we may easily conclude, as for the standard Runge-Kutta case [10], that B-stability implies AN-stability (which also implies A-stability).

We are now in position to prove the converse result of the previous theorem.

Theorem 3.5. *Let us consider a non-confluent ARK method (2.3) (where $c_i \neq c_j$ for $i \neq j$). Then the concepts of AN-stability, B-stability and algebraic stability are equivalent.*

Proof: According to the previous results, we only need to prove that AN-stability implies algebraic stability.

Let us first note that, if we consider, in the proof of Theorem 3.3, $v_0 = 1$ and $w_i^{[\nu]} = \xi_i^{[\nu]} v_i$ we have $v = R(\xi)$. Then, following the same steps of that proof, and noticing that $\xi_i^{[\nu]}$ could not be real, we may conclude that

(3.9)

$$|R(\xi)|^2 = 1 + 2\sum_{\nu=1}^{N}\sum_{i=1}^{s} b_i^{[\nu]}\text{Re}(\xi_i^{[\nu]})|Y_{n,i}|^2 - \sum_{\nu,\mu=1}^{N}\sum_{i,j=1}^{s} m_{ij}^{[\nu\mu]}\overline{\xi_i^{[\nu]}}\,\overline{Y_{n,i}}\xi_j^{[\mu]}Y_{n,j},$$

where $Y_{n,i}$ is the solution of the algebraic equations in (3.4) with $y_n = 1$.

The method is non-confluent and so $\xi_i^{[\nu]}$, $i = 1, ..., s$, $\nu = 1, ..., N$, can be choose arbitrarily in $\mathbb{C}_0^-$. Let us consider $\xi_i^{[\nu]} = -\epsilon$ and $\xi_j^{[\mu]} = 0$, for $j \neq i$, $\mu = 1, ..., N$, so that the matrix Ξ given in (3.6) is regular. If we substitute these values in (3.9) we obtain

$$|\mathrm{Re}(\xi)|^2 - 1 = -2\epsilon b_i^{[\nu]}|Y_{n,i}|^2 - m_{ii}^{[\nu\nu]}\epsilon^2|Y_{n,i}|^2.$$

Choosing an ϵ sufficiently small we conclude that AN-stability implies $b_i^{[\nu]} \geq 0$. With the same arguments we prove that AN-stability is a sufficient condition to $B^{[\nu]} \geq 0$, $\nu = 1, ..., N$.

To prove the non-negativity of $M^{[\nu\mu]}$, let us consider $\eta_j^{[\nu]}$, $j = 1, ..., s$, $\nu = 1, ..., N$, arbitrary real numbers and $\xi_j^{[\nu]} = \epsilon\eta_j^{[\nu]}$ pure imaginary numbers. If we substitute in (3.9) we obtain

$$|\mathrm{Re}(\xi)|^2 - 1 = -\epsilon^2 \sum_{\nu,\mu=1}^{N} \sum_{i,j=1}^{s} m_{ij}^{[\nu\mu]}\eta_i^{[\mu]}\eta_j^{[\nu]}\overline{Y_{n,i}}\ \overline{Y_{n,j}}.$$

It is also possible to choose $\xi_j^{[\nu]}$ so that $Y_{n,j} = 1 + \mathcal{O}(\epsilon)$, as $\epsilon \to 0$, for all j and ν. By hypothesis, and taking ϵ small enough, we conclude that $M^{[\nu\mu]}$ must be non-negative. $\square$

Note that B-stable ARK methods suffer a serious practical disadvantage. In fact, as we may easily see, these methods are always implicit, which means that we cannot find any B-stable Implicit-Explicit method [2].

In the next section we will present a class of B-stable fractional step Runge-Kutta methods of order 2. These methods are a particular case of B-stable ARK methods and have some good numerical features.

4. A class B-stable fractional step Runge-Kutta methods

The notion of algebraic stability can be adapted to FSRK methods in the following way.

Definition 4.1. If an FSRK method (2.7) is such that the matrices

(i) $B := \mathrm{diag}\left(b_1^{[\theta_1]}, \ldots, b_s^{[\theta_s]}\right)$ and

(ii) $M := BA + A^T B - bb^T$

are non-negative then the method is said to be algebraically stable.

Taking into account the special structure of these methods, the following corollary results immediately from Theorem 3.3 and Theorem 3.5.

Corollary 4.2. *A sufficient condition for an FSRK method (2.3) to be B-stable is to be algebraically stable. For non-confluent methods, the converse result is also true.*

Let us now find a class of B-stable FSRK methods (2.7) of order 2 with $s = 3$ and such that the corresponding ARK method has $N = 2$ levels. Without loss of generality we may consider $\theta = [1, 2, 1]^T$. The order conditions are the following [1].

Order 1: For the consistency of the method we must impose

$$\sum_{i:\theta_i=\nu} b_i^{[\theta_i]} = 1, \qquad \nu = 1, 2.$$

In our case these conditions correspond to

$$b_3^{[1]} = 1 - b_1^{[1]}, \quad b_2^{[2]} = 1.$$

Order 2: To obtain FSRK methods of order 2 the coefficients of the method must satisfy

$$\sum_{i:\theta_i=\nu} \sum_{\substack{j:j\le i \\ \theta_j=\mu}} b_i^{[\theta_i]} a_{ij}^{[\theta_j]} = \frac{1}{2}, \qquad \nu, \mu = 1, 2.$$

We may easily conclude that these conditions imply that

$$a_{21}^{[2]} = a_{22}^{[2]} = \frac{1}{2}, \quad a_{32}^{[2]} = \frac{1}{2(1 - b_1^{[1]})}, \quad a_{31}^{[1]} = a_{32}^{[2]}(1 - 2a_{11}^{[1]} b_1^{[1]}) - a_{33}^{[1]}.$$

Thus, in a FSRK method (2.7) of order 2 with $s = 3$ and $\theta = [1, 2, 1]^T$, the coefficients $a_{11}^{[1]}$, $a_{33}^{[1]}$ and $b_1^{[1]}$ remain as free parameters.

For the method to be B-stable, we must also impose the the conditions given in the Definition 4.1. We may easily prove that these two conditions imply that $b_1^{[1]} = \frac{1}{2}$ and that $a_{11}^{[1]} = a_{33}^{[1]} = c$, with c a free parameter such that $c \ge \frac{1}{4}$. So, the class of FSRK methods (2.7) of order 2 with $s = 3$ and $\theta = [1, 2, 1]^T$ is of the form

$$\begin{array}{c|ccc} & 1 & 2 & 1 \\ \hline & c & 0 & 0 \\ & \frac{1}{2} & \frac{1}{2} & 0 \\ & 1-2c & 1 & c \\ \hline & \frac{1}{2} & 1 & \frac{1}{2} \end{array}, \qquad c \ge \tfrac{1}{4}$$

We denote the methods of this class by $\mathrm{FSRK}_h[c]$, with $c \ge 1/4$ and $h \in \mathbb{R}$.

Using composition methods, we may describe a procedure that enables us to construct higher order B-stable numerical methods. Let us consider $c = 1/4$. Then we obtain the numerical method $\mathrm{FSRK}_h[1/4]$ which is of the form (2.2), with $\alpha = 1/2$, i.e.

$$\mathrm{FSRK}_h[1/4] = \psi^{\mathrm{MP}}_{h/2, f^{[1]}} \circ \psi^{\mathrm{MP}}_{h, f^{[2]}} \circ \psi^{\mathrm{MP}}_{h/2, f^{[1]}}.$$

Note that this method is a symmetric method of order two. According to [12, Theorem 22], the composition

$$(\psi_{w_1 h})^{m_1} \circ (\psi_{w_2 h})^{m_2} \circ (\psi_{w_1 h})^{m_1},$$

of a symmetric method ψ_h of order $2k$ is symmetric and has has order $2k+2$, provided that

$$w_1 = (2m_1 - (2m_1 m_2^{2k})^{1/(2k+1)})^{-1}, \qquad w_2 = (1-2m_1 w_1)/m_2.$$

In our case, the method

$$\mathrm{FSRK}_{w_2 h}[1/4] \circ \mathrm{FSRK}_{w_1 h}[1/4] \circ \mathrm{FSRK}_{w_2 h}[1/4],$$

with $w_1 = (2-2^{1/3})^{-1}, w_2 = 1-2w_1$, is symmetric and has order 4 and is B-stable, since the composition of B-stable methods is a B-stable method.

In spite of the fact that B-stable FSRK methods are (diagonally) implicit, if the splitting (2.1) is done in an appropriate manner, the resulting method could have great computational advantages. In some special cases we may obtain an "almost explicit" B-stable method, i.e. a B-stable method with the computational efficiency similar to an explicit solver. To give an example, let us consider the Robertson chemical reaction equation [10]

$$\begin{cases} y_1' &= -0.04y_1 + 10^4 y_2 y_3, \\ y_2' &= 0.04y_1 - 10^4 y_2 y_3 - 3\times 10^7 y_2^2, \\ y_3' &= 3\times 10^7 y_2^2. \end{cases} .$$

If we consider this system in the form (2.1) where

$$f^{[1]}(y) = \begin{bmatrix} -0.04y_1 \\ 0.04y_1 - 3\times 10^7 y_2^2 \\ 3\times 10^7 y_2^2 \end{bmatrix}$$

and

$$f^{[2]}(y) = 10^4 \begin{bmatrix} y_2 y_3 \\ -\, y_2 y_3 \\ 0 \end{bmatrix},$$

and integrate this problem using the $\mathrm{FSRK}_h[1/4]$ method we do not need to use any Newton iterations. In fact, the non-linear equation can be explicitly solved.

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