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**Abstract**

Positivity results are derived for explicit two-step methods formulated in linear multistep form and in one-leg form. It turns out that the latter formulation allows a slightly larger step size with respect to positivity.

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## 1 Introduction

We consider the initial value problem for a positive system of ordinary differential equations (ODEs) in $\mathbb{R}^m$

$$\begin{aligned} \boldsymbol{w}'(t) &= \boldsymbol{F}(t, \boldsymbol{w}(t)), \\ \boldsymbol{w}(0) &= \boldsymbol{w}_0 \geq 0. \end{aligned}$$

With positivity (actually, non-negativity) we mean that the solution vector $\boldsymbol{w}(t) \geq 0$, $\forall\, t > 0$ if $\boldsymbol{w}_0 \geq 0$. Here, and in the sequel, such inequalities are to be understood componentwise. For such systems of ODEs we will study whether we can obtain a similar property for the numerical solutions $\boldsymbol{W}_n \approx \boldsymbol{w}(t_n)$, $t_n = n\Delta t$, $\Delta t$ being the time step. In [4], the related concept of monotonicity with semi-norms for linear multistep methods has been studied. Here we focus on positivity and adapt the results obtained in [4]. In Section 2 we will present an extension in the case of explicit two-step methods with forward Euler start-up (to compute $\boldsymbol{W}_1$), and we will point out the best method with respect to positivity, i.e. $\boldsymbol{W}_n \geq 0$ for $n \geq 1$, whenever $\boldsymbol{W}_0 \geq 0$. In Section 3 we consider the corresponding one-leg formulation and show that this allows a slightly larger step size.

## 2 Positivity for linear two-step methods

Consider the following explicit linear two-step scheme

$$\boldsymbol{W}_{n+2} = \sum_{j=0}^{1} \Big[ -\alpha_j \boldsymbol{W}_{n+j} + \beta_j \,\Delta t\, \boldsymbol{F}(t_{n+j}, \boldsymbol{W}_{n+j}) \Big]. \tag{1a}$$

Observe that the freedom in scaling the coefficients has been used to set the coefficient in front of $\boldsymbol{W}_{n+2}$ equal to 1. In the one-leg formulation we will use a different scaling.

The scheme (1a) is of second-order accuracy if

$$\alpha_0 = 1 - \xi,\ \alpha_1 = \xi - 2,\ \beta_0 = \frac{\xi}{2} - 1,\ \beta_1 = \frac{\xi}{2} + 1, \tag{1b}$$

where $\xi$ is a free parameter. We note that the scheme is zero-stable (stable for the trivial equation $\boldsymbol{w}'(t) = \boldsymbol{0}$, see [5]) if the condition $-1 \le \alpha_0 < 1$ is satisfied, i.e. if $0 < \xi \le 2$. In the remainder of this paper we shall always deal with methods that are second-order accurate and zero-stable. In [4], both implicit and explicit methods have been analyzed. In this section we will extend the results obtained in that paper for the explicit methods. For monotonicity results with higher-order methods, we refer to [2, 3].

Following Shu [7], the step in (1a) is written as a linear combination of scaled forward Euler steps yielding

$$\boldsymbol{W}_{n+2} = -\sum_{j=0}^{1} \alpha_j \Big[ \boldsymbol{W}_{n+j} + c_j \Delta t\, \boldsymbol{F}(t_{n+j}, \boldsymbol{W}_{n+j}) \Big], \quad c_j = -\frac{\beta_j}{\alpha_j}. \tag{2}$$

We define $\Delta t_{FE}$ to be the largest time step for which the forward Euler method, starting from a positive value, yields a positive result, i.e.

$$\boldsymbol{v} + \Delta t \boldsymbol{F}(t, \boldsymbol{v}) \ge 0 \quad \text{for all} \quad \boldsymbol{v} \ge 0,\ \ t \ge 0,\ \ 0 \le \Delta t \le \Delta t_{FE}. \tag{3}$$

Then, if

$$\beta_j \ge 0 \ \text{ and } \ \alpha_j \le 0, \ \text{ i.e. } \ c_j \ge 0, \ \text{ for } j = 0, 1, \tag{4}$$

the terms within the square brackets in (2) are non-negative under the step size restriction $0 \le c_j \Delta t \le \Delta t_{FE}$, $j = 0, 1$. Therefore, $\boldsymbol{W}_{n+2} \ge 0$ for all $\Delta t \le \min(\frac{1}{c_0}, \frac{1}{c_1}) \Delta t_{FE}$, for *arbitrary* values of $\boldsymbol{W}_0, \boldsymbol{W}_1, \cdots, \boldsymbol{W}_{n+1} \ge 0$.

However, for the class of explicit second-order two-step methods, condition (4) for $\beta_0$ leads to $\xi \ge 2$. Combining this with the zero-stability requirement $0 < \xi \le 2$ gives $\xi = 2$ as the only possible value. This, however, results in $c_1 = \infty$ and hence $\Delta t \le 0$. Indeed, for $\xi = 2$ we obtain

$$\boldsymbol{W}_{n+2} = \Big[ \boldsymbol{W}_n - \boldsymbol{W}_{n+1} \Big] + \Big[ \boldsymbol{W}_{n+1} + 2\Delta t \boldsymbol{F}(t_{n+1}, \boldsymbol{W}_{n+1}) \Big].$$

Although the second term gives a positive contribution for $\Delta t \le \frac{1}{2} \Delta t_{FE}$, the first term can be negative for arbitrary positive $\boldsymbol{W}_n$ and $\boldsymbol{W}_{n+1}$ which may result in $\boldsymbol{W}_{n+2} < 0$.

Fortunately, if we consider appropriate starting conditions, a positive result can be obtained [4, 3]. If $\boldsymbol{W}_1$ is obtained by the forward Euler method, i.e.

$$\boldsymbol{W}_1 = \boldsymbol{W}_0 + \Delta t \boldsymbol{F}(t_0, \boldsymbol{W}_0), \tag{5}$$

we have $\boldsymbol{W}_1 \geq 0$ for all $\Delta t \leq \Delta t_{FE}$ (see (3)). By introducing a non-negative parameter $\theta$, which is specified later, and subsequently subtracting and adding $\theta^j \boldsymbol{W}_{n+2-j}, j = 1, 2, \cdots, n+1$, in (1a), in which the added terms with $j = 1, 2, \cdots, n$ are again written in the form of (1a), we arrive at

$$\begin{aligned} \boldsymbol{W}_{n+2} = \ & (-\alpha_1 - \theta)\boldsymbol{W}_{n+1} + \beta_1 \Delta t\, \boldsymbol{F}_{n+1} \\ & + \sum_{j=0}^{n-1} \theta^j \Big[ (-\alpha_0 - \theta\alpha_1 - \theta^2)\boldsymbol{W}_{n-j} + (\beta_0 + \theta\beta_1)\Delta t \boldsymbol{F}_{n-j} \Big] \\ & + \ \theta^{n-1} \Big[ \theta^2 \boldsymbol{W}_1 - \theta\alpha_0 \boldsymbol{W}_0 + \theta\beta_0 \Delta t \boldsymbol{F}_0 \Big], \qquad n \geq 0, \end{aligned} \tag{6}$$

where $\boldsymbol{F}_j$ denotes $\boldsymbol{F}(t_j, \boldsymbol{W}_j)$. Since $\boldsymbol{W}_1$ was calculated by the forward Euler method and $\alpha_1 = -1 - \alpha_0$ (see (1b)), this relation can be written as

$$\begin{aligned} \boldsymbol{W}_{n+2} = \ & (-\alpha_1 - \theta)\boldsymbol{W}_{n+1} + \beta_1 \Delta t\, \boldsymbol{F}_{n+1} \\ & + \sum_{j=0}^{n-1} \theta^j \Big[ (1 - \theta)(\theta - \alpha_0)\boldsymbol{W}_{n-j} + (\beta_0 + \theta\beta_1)\Delta t \boldsymbol{F}_{n-j} \Big] \\ & + \ \theta^{n} \Big[ (\theta - \alpha_0) \boldsymbol{W}_0 + (\theta + \beta_0) \Delta t \boldsymbol{F}_0 \Big], \qquad n \geq 0. \end{aligned}$$

Considering this step as a linear combination of scaled forward Euler steps, we see that $\boldsymbol{W}_{n+2} \geq 0$ if all coefficients are non-negative, i.e.

$$-\alpha_1 - \theta \geq 0, \ \ \beta_1 \geq 0, \ \ (1-\theta)(\theta - \alpha_0) \geq 0, \ \ \beta_0 + \theta\beta_1 \geq 0, \ \ \theta - \alpha_0 \geq 0, \ \ \theta + \beta_0 \geq 0. \tag{7}$$

These conditions imply the step size restriction $\Delta t \leq \gamma(\theta)\Delta t_{FE}$, where

$$\gamma(\theta) = \min\left( \frac{-\alpha_1 - \theta}{\beta_1}, \ \frac{(1-\theta)(\theta - \alpha_0)}{\beta_0 + \theta\beta_1}, \ \frac{\theta - \alpha_0}{\theta + \beta_0} \right) =: \min\left(A(\theta), B(\theta), C(\theta)\right). \tag{8}$$

Obviously, the larger $\gamma(\theta)$, the better are the positivity properties of the scheme.

The conditions (7) define an eligible $\theta$-interval, viz. $\theta \in [\theta_{min}, \theta_{max}]$, where

$$\begin{aligned} \theta_{min} &= \max(\alpha_0, -\tfrac{\beta_0}{\beta_1}, -\beta_0) = -\beta_0, \\ \theta_{max} &= \min(-\alpha_1, 1). \end{aligned}$$

Observe that $A(\theta)$, $B(\theta)$ and $C(\theta)$ are monotonic decreasing functions of $\theta$ (recall the condition $0 < \xi \leq 2$). Therefore, we obtain the maximal $\gamma(\theta)$-value

$$\gamma_{max} \ = \ \min\left(A(\theta_{min}), \ B(\theta_{min}), \ C(\theta_{min})\right) \ = \ \begin{cases} B(\theta_{min}) = \frac{\xi}{2-\xi} & \text{if } 0 < \xi \leq \frac{2}{3}, \\ A(\theta_{min}) = \frac{2-\xi}{2+\xi} & \text{if } \frac{2}{3} \leq \xi \leq 2. \end{cases} \tag{9}$$

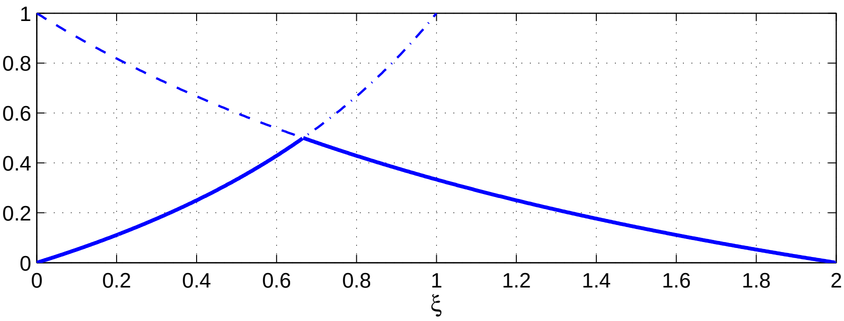


Figure 1: $\gamma_{max}$ (solid), $A(\theta_{min})$ (dashed), and $B(\theta_{min})$ (dash-dotted) as functions of $\xi$.

The result is plotted in Figure 1. The ascending part of the $\gamma_{max}$-curve (i.e. for $0 < \xi < \frac{2}{3}$) is an extension to the work in [4]. We note that in that paper only the minimum of $A(\theta)$ and $B(\theta)$ was considered in (8), leading to a different value of $\theta_{min}$. The forward Euler starting procedure (5) was introduced afterwards, but this does not lead to a positivity result for $0 < \xi < \frac{2}{3}$.

From Figure 1 we see that, within the class of explicit second-order two-step method, the optimal method with respect to positivity is the $\xi = \frac{2}{3}$ method (known as the extrapolated BDF2 method [5]). The resulting value for $\gamma_{max}$ is $\frac{1}{2}$.

**Remark**. In (6), the sequence of subtracting and adding $\theta^j \boldsymbol{W}_{n+2-j}$ was performed until $j = n+1$. In [4] these terms were subtracted and added up to $j = n$. It has been proved [6] that the latter choice has no advantages compared with the choice made in (6), i.e., does not lead to a more relaxed condition on $\Delta t$. The proof is rather lengthy and technical and therefore is not included in this paper.

## 3 Positivity for one-leg methods

One-leg schemes were introduced by Dahlquist [1] to facilitate the analysis of linear multistep methods. Therefore, it is of interest to study the positivity properties of methods when formulated in the one-leg form. Similar to the preceding section, we will consider explicit methods. We will see that the results are slightly better than those derived for the linear multistep formulation.

A natural scaling for one-leg methods is to require $\beta_0 + \beta_1 = 1$. Starting from the linear multistep formulation (1) we multiply the coefficients by a factor $\frac{1}{\xi}$ to obtain

$$\alpha_2 \boldsymbol{W}_{n+2} = \sum_{j=0}^{1} \Big[ -\alpha_j \boldsymbol{W}_{n+j} + \beta_j \, \Delta t \, \boldsymbol{F}(t_{n+j}, \boldsymbol{W}_{n+j}) \Big], \tag{10a}$$

where

$$\alpha_0 = \frac{1}{\xi} - 1, \;\; \alpha_1 = 1 - \frac{2}{\xi}, \;\; \alpha_2 = \frac{1}{\xi}, \;\; \beta_0 = \frac{1}{2} - \frac{1}{\xi}, \;\; \beta_1 = \frac{1}{2} + \frac{1}{\xi}. \tag{10b}$$

Since $\xi > 0$ we have

$$0 < \alpha_2 = -(\alpha_1 + \alpha_0). \tag{11}$$

The one-leg form of (10a) reads

$$\begin{aligned} \alpha_2 \boldsymbol{W}_{n+2} &= -\alpha_1 \boldsymbol{W}_{n+1} - \alpha_0 \boldsymbol{W}_n + \Delta t \boldsymbol{F}\left(\bar{t}, \overline{\boldsymbol{W}}_{n+2}\right), \\ \overline{\boldsymbol{W}}_{n+2} &= \beta_1 \boldsymbol{W}_{n+1} + \beta_0 \boldsymbol{W}_n, \end{aligned} \tag{12}$$

where $\bar{t} = \beta_1 t_{n+1} + \beta_0 t_n = t_n + \beta_1 \Delta t$. This one-leg formulation is second-order accurate if the coefficients satisfy (10b).

Let us define

$$\boldsymbol{V}_n = \boldsymbol{W}_n - \theta \boldsymbol{W}_{n-1}, \quad \theta \in [0,1), \quad n \geq 1. \tag{13}$$

Furthermore, we introduce the coefficients

$$\begin{aligned} &\alpha_1^* = -\alpha_1 - \alpha_2\theta, \quad \alpha_2^* = -\alpha_0 - \alpha_1\theta - \alpha_2\theta^2 = (1-\theta)(\alpha_2\theta - \alpha_0), \\ &\beta_1^* = \beta_1, \qquad\qquad\quad \beta_2^* = \beta_0 + \beta_1\theta. \end{aligned} \tag{14}$$

The parameter $\theta$ in (13) and (14) will be chosen such that the coefficients in (14) satisfy

$$\alpha_j^* \geq 0, \quad \beta_j^* \geq 0, \quad j = 1, 2. \tag{15}$$

Assuming positive starting values

$$\boldsymbol{V}_1 \geq 0 \text{ and } \boldsymbol{W}_1 \geq 0, \tag{16}$$

we have the following theorem.

**Theorem 1.** *Suppose that* $\Delta t \leq \mathcal{C}\Delta t_{FE}$*, with* $\mathcal{C} = \min\left(\frac{\alpha_1^*}{\beta_1^*}, \frac{\alpha_2^*}{\beta_2^*}\right)$*, and* $\theta$ *is such that the conditions (15) and (16) are satisfied. Then* $\boldsymbol{V}_n \geq 0$ *and* $\boldsymbol{W}_n \geq 0$ *for all* $n \geq 1$*.*

*Proof.* The formulae (12)–(13) give

$$\alpha_2 \boldsymbol{V}_{n+2} = \alpha_1^* \boldsymbol{V}_{n+1} + \alpha_2^* \boldsymbol{W}_n + \Delta t \boldsymbol{F}\left(\bar{t}, \overline{\boldsymbol{W}}_{n+2}\right), \tag{17}$$

$$\overline{\boldsymbol{W}}_{n+2} = \beta_1^* \boldsymbol{V}_{n+1} + \beta_2^* \boldsymbol{W}_n. \tag{18}$$

Adding $\mathcal{C}\overline{\boldsymbol{W}}_{n+2}$ to both sides in equation (17) we obtain

$$\alpha_2 \boldsymbol{V}_{n+2} = (\alpha_1^* - \mathcal{C}\beta_1^*)\boldsymbol{V}_{n+1} + (\alpha_2^* - \mathcal{C}\beta_2^*)\boldsymbol{W}_n + \mathcal{C}\overline{\boldsymbol{W}}_{n+2} + \Delta t \boldsymbol{F}\left(\bar{t}, \overline{\boldsymbol{W}}_{n+2}\right).$$

The coefficients in this relation are non-negative, due to the definition of $\mathcal{C}$ and (11). Therefore, $\boldsymbol{V}_{n+2} \geq 0$ if

$$\boldsymbol{V}_{n+1} \geq 0, \quad \boldsymbol{W}_n \geq 0, \quad \mathcal{C}\overline{\boldsymbol{W}}_{n+2} + \Delta t \boldsymbol{F}\left(\bar{t}, \overline{\boldsymbol{W}}_{n+2}\right) \geq 0. \tag{19}$$

The term $\mathcal{C}\overline{\boldsymbol{W}}_{n+2} + \Delta t \boldsymbol{F}\left(\bar{t}, \overline{\boldsymbol{W}}_{n+2}\right)$ can be seen as a scaled forward Euler step. Thus, it is non-negative if $\overline{\boldsymbol{W}}_{n+2} \geq 0$ and $\Delta t \leq \mathcal{C}\Delta t_{FE}$. From (18) and (15) we see that $\overline{\boldsymbol{W}}_{n+2} \geq 0$ if

$$\boldsymbol{V}_{n+1} \geq 0 \quad \text{and} \quad \boldsymbol{W}_n \geq 0. \tag{20}$$

Combining (19) and (20) we have

$$\boldsymbol{V}_{n+2} \geq 0 \;\text{ if }\; \boldsymbol{V}_{n+1} \geq 0 \;\text{ and }\; \boldsymbol{W}_n \geq 0. \tag{21}$$

By assumption, we know that $\boldsymbol{V}_1 \geq 0$, $\boldsymbol{W}_1 \geq 0$ (see (16)) and $\boldsymbol{W}_0 \geq 0$. Thus, (21) yields $\boldsymbol{V}_2 \geq 0$. As a result, relation (13) gives $\boldsymbol{W}_2 = \boldsymbol{V}_2 + \theta \boldsymbol{W}_1 \geq 0$. Having $\boldsymbol{V}_2 \geq 0$ and $\boldsymbol{W}_1 \geq 0$, we obtain $\boldsymbol{V}_3 \geq 0$ (again by (21)) which results in $\boldsymbol{W}_3 = \boldsymbol{V}_3 + \theta \boldsymbol{W}_2 \geq 0$, etc. for all $n \geq 4$. □

Let us now return to assumption (16) on the starting values. If $\boldsymbol{W}_1$ is calculated by the forward Euler method then we have $\boldsymbol{W}_1 \geq 0$ for all $\Delta t \leq \Delta t_{FE}$. Moreover, $\boldsymbol{V}_1 = \boldsymbol{W}_1 - \theta \boldsymbol{W}_0 = (1-\theta)\boldsymbol{W}_0 + \Delta t \boldsymbol{F}_0 \geq 0$ under the additional step size restriction $\Delta t \leq (1-\theta)\Delta t_{FE}$.

Using the above considerations we can formulate the following theorem on the positivity condition for the one-leg method.

**Theorem 2.** *If $\boldsymbol{W}_1$ is obtained by the forward Euler method (5) and $\theta$ is such that condition (15) is satisfied, then the one-leg method (12) is positive under the step size restriction $\Delta t \leq \gamma^{OL}(\theta)\Delta t_{FE}$ where*

$$\gamma^{OL}(\theta) = \min(\mathcal{C}, 1-\theta) = \min\left(\frac{-\alpha_1 - \alpha_2\theta}{\beta_1}, \frac{(1-\theta)(\alpha_2\theta - \alpha_0)}{\beta_0 + \beta_1\theta}, 1-\theta\right). \tag{22}$$

It is illustrative to compare this $\gamma^{OL}(\theta)$ with the $\gamma(\theta)$ derived in (8): Condition (15) gives $\theta \in [\theta_{min}, \theta_{max}]$, where

$$\begin{aligned} \theta_{min} &= \max(\tfrac{\alpha_0}{\alpha_2}, -\tfrac{\beta_0}{\beta_1}) = -\tfrac{\beta_0}{\beta_1}, \\ \theta_{max} &= \min(-\tfrac{\alpha_1}{\alpha_2}, 1). \end{aligned}$$

Observe that the terms in the minimum function in (22) are monotonic decreasing functions of $\theta$. Therefore, the optimal $\gamma^{OL}(\theta)$-value is obtained at $\theta = \theta_{min} = \frac{2-\xi}{2+\xi}$ and is given by

$$\gamma^{OL}_{max} = \min\left(\frac{2(1+\xi)(2-\xi)}{(2+\xi)^2}, \frac{2\xi}{2+\xi}\right). \tag{23}$$

The result is plotted in Figure 2. From this figure we see that the best method with respect to positivity is no longer the method with $\xi = \frac{2}{3}$. The optimal method with respect to positivity is now the method with $\xi = \frac{1}{4}(\sqrt{17}-1) \approx 0.78$. The corresponding $\gamma^{OL}_{max}$ is then $\frac{1}{2}(\sqrt{17}-3) \approx 0.56$. Comparing (9) and (23) we see that the one-leg method allows a slightly larger time step than the linear two-step method.

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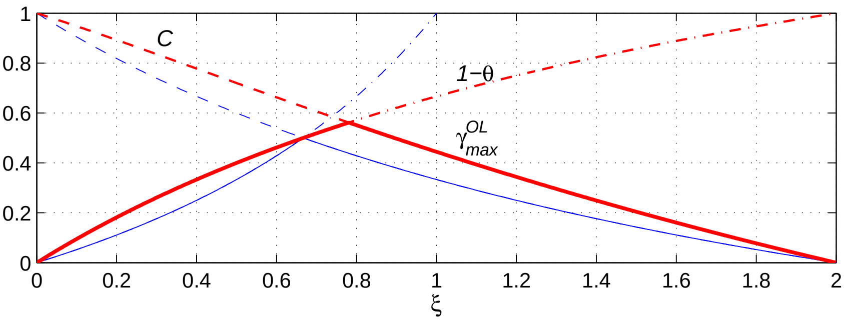


Figure 2: Step size restriction for positivity of the one-leg methods (thick lines) and of the linear two-step methods (thin lines, obtained from Figure 1).

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