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Monotonicity for Time Discretizations

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Abstract

These notes contain an extended summary of a lecture given at the 20th Biennial Conference on Numerical Analysis, Dundee, 2003. This review is largely based on material from [7, 8], where additional results and a more precise presentation can be found.

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1 Introduction

The preservation of monotonicity properties – like maximum principles and positivity – is often essential for numerical schemes to approximate non-smooth solutions in a qualitatively correct manner. In these notes a review is given of monotonicity results for time stepping with Runge-Kutta and linear multistep methods.

We consider an ODE system in $\mathbb{R}^m$

$$w'(t) = F(w(t)), \quad w(0) = w_0 . \tag{1.1}$$

In the applications this will originate from a PDE after suitable spatial discretization. Then approximations $w_n \approx w(t_n)$, $t_n = n\Delta t$, are obtained by a time stepping method with step size Δt.

In these notes we shall deal with the property

$$\|w_n\| \le \|w_0\| \qquad \text{for } \; n \ge 1\,, \; w_0 \in \mathbb{R}^m, \tag{1.2}$$

where $\|\cdot\|$ is a given semi-norm. This may be, for example, the maximum-norm or the total variation over the components. In the latter case (1.2) is called the TVD property (total variation diminishing). It is assumed that

$$\|v + \Delta t\, F(v)\| \le \|v\| \qquad \text{for } \; 0 < \Delta t \le \Delta t_{FE}\,, \; v \in \mathbb{R}^m, \tag{1.3}$$

where Δt_{FE} can be viewed as the maximal step size for the forward Euler method. Condition (1.3) is often easy to verify [5, 8]. The goal is to specify for higher-order methods the *monotonicity threshold* $C > 0$ such that (1.2) holds whenever $\Delta t \le C\, \Delta t_{FE}$.

Related monotonicity properties are *positivity* ($w_n \ge 0$ whenever $w_0 \ge 0$) and the *comparison principle* ($w_n \ge v_n$ whenever $w_0 \ge v_0$), with inequalities for vectors component-wise. Properties like these and (1.2) are often called *monotonicity*. The main motivation for wanting such properties is to avoid oscillations in the numerical solutions and to prevent over- and undershoots.

Example 1.1 Before considering general results for time stepping methods, in the Sections 2, 3 and 4, let us first consider some simple examples.

The implicit Euler method

$$w_n = w_{n-1} + \Delta t\, F(w_n) \tag{1.4}$$

is unconditionally monotone, $C_{BE} = \infty$. This is easily seen from

$$\Big(1 + \frac{\Delta t}{\Delta t_{FE}}\Big) w_n \;=\; w_{n-1} + \frac{\Delta t}{\Delta t_{FE}}\Big(w_n + \Delta t_{FE}\, F(w_n)\Big)$$

with application of the triangle inequality to the right-hand side.

The implicit trapezoidal rule

$$w_n = w_{n-1} + \frac{1}{2}\,\Delta t\, F(w_{n-1}) + \frac{1}{2}\,\Delta t\, F(w_n) \tag{1.5}$$

has threshold factor $C_{ITR} = 2$; the method consists of a forward Euler half-step followed by a backward Euler half-step (with $\frac{1}{2}\Delta t$).

The explicit trapezoidal rule (modified Euler)

$$\overline{w}_n = w_{n-1} + \Delta t\, F(w_{n-1})\,, \qquad w_n = w_{n-1} + \frac{1}{2}\,\Delta t\, F(w_{n-1}) + \frac{1}{2}\,\Delta t\, F(\overline{w}_n) \tag{1.6}$$

has threshold factor $C_{ETR} = 1$. This becomes more apparent by writing the second stage as

$$w_n = \frac{1}{2}\, w_{n-1} + \frac{1}{2}\,\Big(\overline{w}_n + \Delta t\, F(\overline{w}_n)\Big)\,.$$

From these simple examples we see that methods have to be rewritten sometimes in a form that is more convenient to make the monotonicity apparent. More importantly, we see that there is no direct relation with the usual stability properties of the methods. After all, the implicit trapezoidal rule is A-stable, whereas its explicit counterpart (1.6) is only conditionally stable. In fact, the backward Euler method will turn out to be the only well-known method with threshold value $C = \infty$.

Example 1.2 To illustrate the relevance of monotonicity, we consider the Buckley-Leverett equation

$$u_t + f(u)_x = 0\,, \qquad f(u) = \frac{3u^2}{3u^2 + (1-u)^2}\,,$$

for $t \ge 0$, $0 \le x \le 1$, with inflow condition $u(0,t) = 1$ and an initial block-function: $u(x,0)$ is zero on $(0, \frac{1}{2}]$, one on $(\frac{1}{2}, 1]$. We use a fixed grid with mesh width $\Delta x = 5 \cdot 10^{-3}$ and a flux-limited spatial discretization (van Leer type; see [8] for the semi-discrete form). This then defines our ODE system. The PDE solution consists of two shocks followed by rarefaction waves; in the semi-discrete solution the shocks are slightly diffused, over a few grid cells.

The implicit BDF2 scheme

$$w_n = \frac{4}{3} w_{n-1} - \frac{1}{3} w_{n-2} + \frac{2}{3} \Delta t\, F(w_n) \tag{1.7}$$

has order 2 and it is A-stable, that is, unconditionally stable in a von Neumann analysis. Its explicit counterpart, the extrapolated BDF2 scheme

$$w_n = \frac{4}{3}w_{n-1} - \frac{1}{3}w_{n-2} + \frac{4}{3}\Delta t\, F(w_{n-1}) - \frac{2}{3}\Delta t\, F(w_{n-2}) \tag{1.8}$$

also has order 2. It is stable with the present spatial discretization for Courant numbers up to 0.5, approximately. As we shall see below, the two schemes have approximately the same monotonicity threshold.

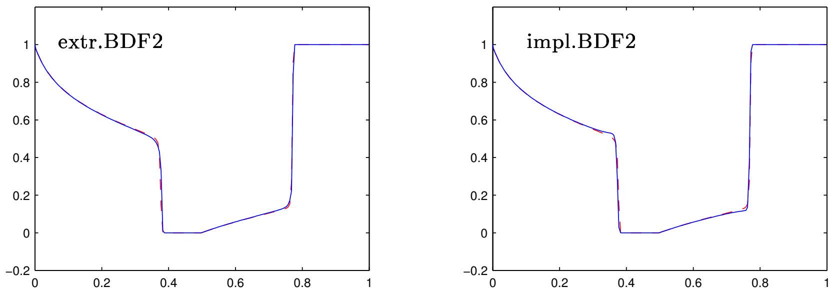

Figure 1: BDF2 solutions at $t = 1/4$ for the Buckley-Leverett equation with $\Delta t = 1/800$. The dashed line is a time-accurate semi-discrete solution ($\Delta x = 5 \cdot 10^{-3}$).

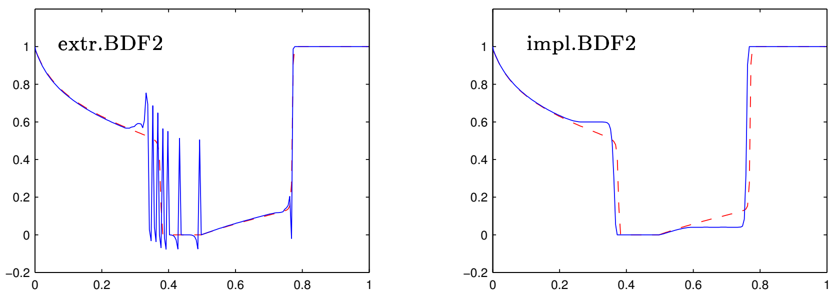

Figure 2: BDF2 solutions at $t = 1/4$ for the Buckley-Leverett equation with $\Delta t = 1/400$. The dashed line is a time-accurate semi-discrete solution ($\Delta x = 5 \cdot 10^{-3}$).

Numerical solutions are given in the Figures 1 and 2. Let us first consider the results with $\Delta t = \frac{1}{800}$. Then both methods give results close to the exact semi-discrete solution. Next we take $\Delta t = \frac{1}{400}$. Then the explicit scheme is becoming unstable. However, also the (unconditionally stable) implicit scheme gives bad results; we now have a wrong location and height of the shocks. This is due to *loss of monotonicity*, giving over- and undershoots after the shocks. (Global overshoots would occur with different initial and boundary conditions, e.g., $u(x,0) = 0$, $u(0,t) = \frac{1}{2}$.)

Example 1.3 The standard examples for which monotonicity is relevant arise in hyperbolic conservation laws. To a lesser extend monotonicity is also important for certain parabolic examples. As an illustration consider the Fisher equation

$$u_t = \epsilon u_{xx} + \gamma u(1-u^2)$$

with traveling wave solution $u(x,t) = (1 + e^{\lambda(x-1-\alpha t)})^{-1}$, where $\lambda = \frac{1}{2}\sqrt{2\gamma/\epsilon}$ and $\alpha = \frac{3}{2}\sqrt{2\gamma\epsilon}$. The parameters are taken as $\gamma = \epsilon^{-1} = 100$ and $0 < x < L = 6$,

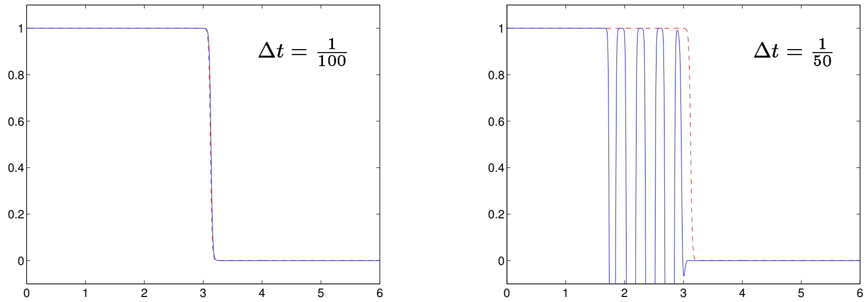

Figure 3: Results for the Fisher equation with the 2-stage Gauss RK method, $\Delta t = 1/100, 1/50$. The dashed line is the exact PDE solution.

$0 < t \leq 1$, with homogeneous Neumann conditions at the boundaries. The mesh width is $\Delta x = 10^{-2}$, and standard second-order differences are used in space.

Then with the explicit Euler method we need approximately $\Delta t \lesssim 1/300$ for monotonicity. Here, we consider the implicit 2-stage Gauss Runge-Kutta method of order 4, and $\Delta t = \frac{1}{100}, \frac{1}{50}$. The results are shown in Figure 3. This method is A-stable but its monotonicity properties are poor ($C = 0$, see [17]) The large oscillations are initiated by small negative solution values that are amplified towards -1 by the reaction term. Because the solution is smooth on fine grids, the threshold $C = 0$ is pessimistic for this example. Nonetheless, it is obvious that the method cannot take large steps without loosing the correct qualitative behaviour.

2 Runge-Kutta methods

The first results on monotonicity were derived for *linear systems* by Bolley & Crouzeix [1] and Spijker [15]. This gives upper bounds for nonlinear systems. For Runge-Kutta methods with s stages and order p, the maximal threshold value $C = C_{RK}$ of explicit methods with $p = s$ is $C_{RK} = 1$. Moreover, among the well-known implicit methods we have unconditional monotonicity, $C_{RK} = \infty$, only for the backward Euler method [1].

Results for *nonlinear systems* were obtained first by Shu & Osher [14], using forms with combinations of Euler steps. For example, a diagonally implicit method can be written as

$$(2.1) \qquad \begin{cases} v_0 = w_{n-1}\,, \\ v_i = \displaystyle\sum_{j=0}^{i-1} \Big(p_{ij}\, v_j + q_{ij} \Delta t\, F(v_j) \Big) + q_{ii} \Delta t\, F(v_i)\,, \qquad i = 1, \ldots, s\,, \\ w_n = v_s\,. \end{cases}$$

If all $p_{ij}, q_{ij} \geq 0$, then

$$\|w_n\| \leq \|w_{n-1}\|$$

holds under step size restriction

$$(2.2) \qquad \Delta t \leq C_{RK}\, \Delta t_{FE}\,, \qquad C_{RK} = \min_{1 \leq j \leq i-1} \left(\frac{p_{ij}}{q_{ij}} \right).$$

Necessary and sufficient conditions were obtained by Kraaijevanger [10] on nonlinear contractivity. A recent result of Ferracina & Spijker [2] shows that with the

Shu-Osher form (2.1) an optimal choice of p_{ij}, q_{ij} leads as well to necessary conditions, also with fully implicit methods. (Note that for a given method in the form of a Butcher tableau, there is some freedom in the choice of the p_{ij}, q_{ij}).

For further results on classes of Runge-Kutta methods with optimal threshold $C_{RK} > 0$, for given p and s, see for instance [2, 4, 5, 8, 10, 16].

Example 2.1 The optimal explicit second-order methods are given by

$$(2.3) \qquad \begin{cases} v_0 \;=\; w_{n-1}\,, \\ v_i \;=\; v_{i-1} + \dfrac{1}{s-1}\,\Delta t\, F(v_{i-1})\,, \qquad i = 1,\ldots,s-1\,, \\ w_n \;=\; \dfrac{1}{s}\, w_{n-1} + \dfrac{s-1}{s}\Big(v_{s-1} + \dfrac{1}{s-1}\,\Delta t\, F(v_{s-1})\Big)\,. \end{cases}$$

This class of methods was derived by Kraaijevanger [9, 10]. The monotonicity threshold factor for these methods is given by

$$C_{RK} = s - 1\,.$$

Kraaijevanger's results were formulated in terms of contractivity. The same methods were derived by Gerisch & Weiner [3] and Spiteri & Ruuth [16], studying related monotonicity properties.

These methods have nicely shaped stability regions (where stability is valid for $z = \Delta t\, \lambda \in \mathcal{S}$ with the scalar test equation $w' = \lambda w$), see Figure 4.

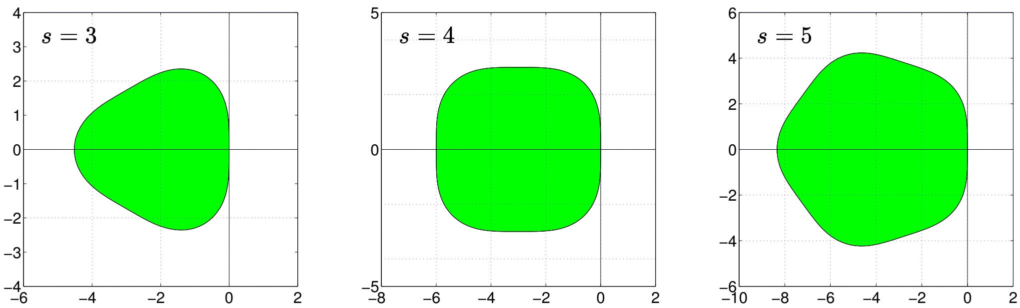

Figure 4: Stability regions $\mathcal{S}$ for the optimal 2nd-order explicit Runge-Kutta methods, $s = 3, 4, 5$.

3 Linear multistep methods with arbitrary starting values

Consider a linear multistep method

$$(3.1) \qquad w_n \;=\; \sum_{j=1}^{k} \Big(a_j w_{n-j} + b_j \Delta t\, F(w_{n-j})\Big) \;+\; b_0 \Delta t\, F(w_n)\,.$$

If all $a_j, b_j \geq 0$, then

$$\|w_n\| \;\leq\; \max_{1\leq j\leq k} \|w_{n-j}\|$$

will hold under the step size restriction

$$(3.2) \qquad \Delta t \;\leq\; C_{LM}\, \Delta t_{FE}\,, \qquad C_{LM} = \min_{1\leq j\leq k} \left(\frac{a_j}{b_j}\right)\,.$$

This result is due to Shu [13] (with $b_0 = 0$), originally in terms of total variations. Related results for linear systems were given in [1] (on positivity), and in [15, 11] (on contractivity).

Using the order conditions, it was shown by Lenferink [11] that the maximal size of the threshold factor C_{LM} for explicit k-step methods of order p is bounded by

$$(3.3)\qquad \begin{cases} C_{LM} \le 1 & \text{if } p = 1\,, \\ C_{LM} \le \frac{k-p}{k-1} & \text{if } p \ge 2\,. \end{cases}$$

The bound for $k = 1$ is attained by the forward Euler method. Optimal higher-order multistep methods have been constructed by Shu [13], Lenferink [11] and Gottlieb et al. [5].

Example 3.1 The explicit 3-step method

$$(3.4)\qquad w_n = \frac{3}{4}\,w_{n-1} + \frac{1}{4}\,w_{n-3} + \frac{3}{2}\,\Delta t\,F(w_{n-1})$$

has order $p = 2$ and $C_{LM} = \frac{1}{2}$. The explicit 4-step method

$$(3.5)\qquad w_n = \frac{8}{9}\,w_{n-1} + \frac{1}{9}\,w_{n-4} + \frac{4}{3}\,\Delta t\,F(w_{n-1})$$

has $p = 2$ and threshold factor $C_{LM} = \frac{2}{3}$. The stability regions of these methods is given in Figure 5.

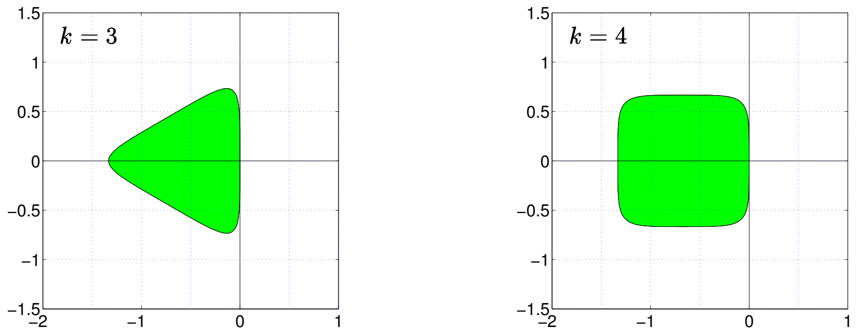

Figure 5: Stability regions $\mathcal{S}$ for the optimal second-order explicit k-step methods, $k = 3, 4$.

4 Linear multistep methods with starting procedures

The above results with arbitrary starting values exclude many schemes that are useful in practice and also may give unnecessary step size restrictions. For example, for explicit methods with $p = k = 2$ we cannot have $C_{LM} > 0$ in view of (3.3). Also, Adams and BDF schemes are excluded. This is due to insistence on *arbitrary* initial vectors, which may give too strong restrictions

For instance, application of the BDF2 method to the trivial problem $w'(t) = 0$ yields

$$w_2 = \frac{4}{3}\,w_1 - \frac{1}{3}\,w_0\,.$$

Obviously, we do not have $\|w_2\| \le \max\big(\|w_0\|, \|w_1\|\big)$ for arbitrary w_0, w_1; but it is also obvious that only $w_1 = w_0$ makes sense here. Therefore we will look at the methods in combination with *starting procedures*. In the following presentation, based on [7], we restrict ourselves to 2-step methods.

The standard form of a 2-step method reads

$$w_n - b_0 \Delta t\, F_n = a_1 w_{n-1} + a_2 w_{n-2} + b_1 \Delta t\, F_{n-1} + b_2 \Delta t\, F_{n-2} \tag{4.1}$$

for $n \ge 2$, with $F_n = F(w_n)$. Let $\theta \ge 0$. By subtracting recursively terms $\theta^j w_{n-j}$ and using (4.1), the multistep scheme can be written out fully up to the starting values,

$$\begin{aligned} w_n - b_0 \Delta t\, F_n &= (a_1 - \theta) w_{n-1} + (b_1 + \theta b_0) \Delta t\, F_{n-1} \\ &+ \sum_{j=2}^{n-2} \theta^{j-2} \Big((a_2 + \theta a_1 - \theta^2) w_{n-j} + (b_2 + \theta b_1 + \theta^2 b_0) \Delta t\, F_{n-j} \Big) \\ &+ \theta^{n-3} \Big((a_2 + \theta a_1) w_1 + (b_2 + \theta b_1) \Delta t\, F_1 + \theta a_2 w_0 + \theta b_2 \Delta t\, F_0 \Big) . \end{aligned}$$

Define

$$C^*_{LM} = \max_{\theta} \, \min \left(\frac{a_1 - \theta}{b_1 + \theta b_0} \,,\, \frac{a_2 + \theta a_1 - \theta^2}{b_2 + \theta b_1 + \theta^2 b_0} \right) , \tag{4.2}$$

where θ is restricted to get nonnegative coefficients. For the starting procedure that yields w_1 we assume that

$$\begin{aligned} \|w_1\| \le M \|w_0\| , \quad \|w_2\| \le M \|w_0\| , \\ \|(a_2 + \theta a_1) w_1 + (b_2 + \theta b_1) \Delta t\, F_1 + \theta a_2 w_0 + \theta b_2 \Delta t\, F_0\| \;\le\; (a_2 + \theta) M \, \|w_0\| , \end{aligned} \tag{4.3}$$

with constant $M \ge 1$. Then we have the following result [7].

Theorem 4.1 *Suppose (4.3) and $\Delta t \le C^*_{LM} \Delta t_{FE}$. Then $\|w_n\| \le M \|w_0\|$ for all $n \ge 1$.*

We note that for any starting procedure, there will be an $M \ge 1$ such that (4.3) is valid with $\Delta t \le C^*_{LM} \Delta t_{FE}$. To get genuine monotonicity, that is, $M = 1$, conditions on the starting procedure and perhaps an additional step size restriction will be needed.

Example 4.2 : Explicit second-order 2-step methods. The explicit methods with $k = p = 2$ form a one-parameter family,

$$w_n \;=\; (2 - \xi)\, w_{n-1} + (\xi - 1)\, w_{n-2} + \;(1 + \tfrac{1}{2}\xi)\, \Delta t\, F_{n-1} + (\tfrac{1}{2}\xi - 1)\, \Delta t\, F_{n-2} . \tag{4.4}$$

The parameter ξ should be in the interval $(0, 2]$ for zero-stability. Interesting examples are $\xi = 1$ (Adams-Bashforth) and $\xi = \frac{2}{3}$ (extrapolated BDF2). Here

$$C^*_{LM} \;=\; \frac{2(1+\xi)(2-\xi)}{(2+\xi)^2} \, .$$

To have $\|w_n\| \le \|w_0\|$ for all n, there can be an additional restriction $\Delta t \le C^0_{LM} \Delta t_{FE}$ for the starting procedure.

A natural starting procedure for (4.4) is given by the forward Euler method,

$$w_1 = w_0 + \Delta t\, F_0 \, .$$

We then have the following result (with $M = M(\xi) \geq 1$):

$$\begin{aligned} \Delta t &\leq C^*_{LM}\,\Delta t_{FE}\,, \quad 0 < \xi \leq 2 \quad \Longrightarrow \quad \|w_n\| \leq M\,\|w_0\|\,, \\ \Delta t &\leq \frac{2-\xi}{2+\xi}\Delta t_{FE}\,, \quad \frac{2}{3} \leq \xi \leq 2 \quad \Longrightarrow \quad \|w_n\| \leq \|w_0\|\,. \end{aligned}$$

Here it should be noted that the restriction for genuine monotonicity ($M = 1$) can be relaxed with more general starting procedures. In numerical experiments (linear advection, Burgers' equation) the restriction $\Delta t \leq C^*_{LM}\,\Delta t_{FE}\,,\ 0 < \xi \leq 2$ was found to be practically relevant. For small $\xi > 0$ the methods often gave inaccurate results due to compression; good numerical results were obtained for $\xi = \frac{2}{3}$ (extrapolated BDF2). See [7] for details.

Example 4.3 : Implicit second-order 2-step methods. The implicit methods with $k = p = 2$ form a two-parameter family,

$$\begin{aligned} w_n - \eta\Delta t\,F_n \;&=\; (2-\xi)w_{n-1} + (\xi-1)w_{n-2} \\ &+ (1 + \tfrac{1}{2}\xi - 2\eta)\Delta t\,F_{n-1} + (\eta + \tfrac{1}{2}\xi - 1)\Delta t\,F_{n-2} \end{aligned} \tag{4.5}$$

with $0 < \xi \leq 2$, $\eta \geq 0$; for A-stability we need $\eta \geq \frac{1}{2}$. Interesting classes are $\xi = \frac{2}{3}$ (BDF2-type) and $\xi = 1$ (2-step Adams type).

Determination of the optimal factors C^*_{LM} is easy numerically. Plots for $\xi = \frac{2}{3}, 1$ as function of η are given in Figure 6. For the familiar implicit BDF2 method ($\xi = \eta = \frac{2}{3}$) we have $C^*_{LM} = \frac{1}{2}$, which is even less than for its explicit counterpart ($\xi = \frac{2}{3}$, $\eta = 0$) where $C^*_{LM} = \frac{5}{9}$. In fact, for these two methods the same thresholds are found if only linear problems are considered [6].

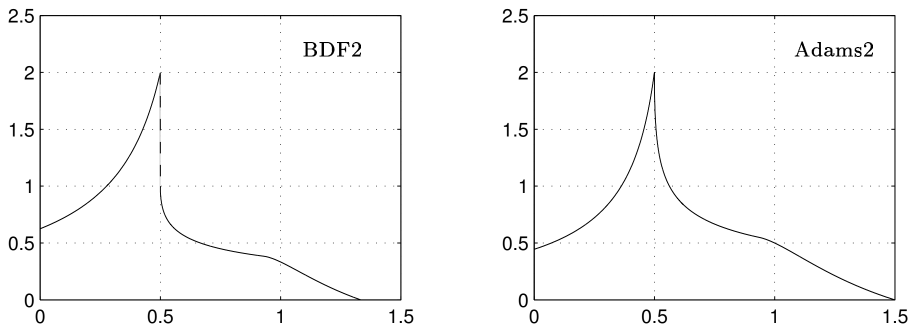

Figure 6: Threshold values C^*_{LM} versus $\eta \in [0, 1.5]$, with $\xi = \frac{2}{3}$ (left) and $\xi = 1$ (right).

Overall, these results are disappointing. The largest numbers $C^*_{LM} = 2$ are found for the values $\eta = \frac{1}{2}$ (similar behaviour with other $\xi \in (0, 2]$). Experimental verification of the curves in Figure 6 is given in [7] for the advection model problem $u_t + u_x = 0$ with first-order spatial differences.

5 Summary

For Runge-Kutta methods the basic monotonicity theory is fairly complete. There is a continuing search for 'optimal' explicit methods and theoretical refinements; see [2, 16, 12] for some recent papers. From a practical point of view, it is important to note that for many standard methods – including implicit (A-stable) methods – quite small step sizes may be needed if monotonicity properties are crucial in an application.

For linear multistep methods, on the other hand, the theory is less well developed. Inclusion of starting procedures in the considerations is needed to get reasonable step size restrictions for monotonicity or boundedness. This inclusion allows statements with classes of methods that are important in practice (such as Adams and BDF-type). In the numerical tests in [7] the standard Adams-Bashforth schemes ($k \leq 3$) and the extrapolated BDF schemes ($k \leq 4$) performed better than special constructed methods [5, 11, 13] with positive coefficients.

Apart from results with 2-step methods, some higher-order methods were analyzed in [7], but each class of methods did require a separate analysis. Optimality statements for general higher-order methods are lacking. Also results for predictor-corrector schemes are at present still absent.

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