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Manh Tuan Hoang and Matthias Ehrhardt

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A general class of second-order L-stable explicit numerical methods for stiff problems

Manh Tuan Hoang[a,*], Matthias Ehrhardt[b,**]

[a] *Department of Mathematics, FPT University, Hoa Lac Hi-Tech Park, Km29 Thang Long Blvd, Hanoi, Viet Nam*
[b] *University of Wuppertal, Chair of Applied and Computational Mathematics, Gaußstrasse 20, 42119 Wuppertal, Germany*

Abstract

In this paper, we propose a simple approach to the construction of a general class of L-stable explicit second-order one-step methods for solving stiff problems. These methods are nonlinear and derive from a novel approximation for the right-hand side functions of differential equations inspired by the nonstandard finite difference methodology introduced by Mickens. Through rigorous mathematical analysis, it is proved that the proposed numerical methods are not only explicit and L-stable, but also convergent of order two. Therefore, they are suitable and efficient to solve stiff problems.

The proposed numerical methods generalize and improve a nonstandard explicit integration scheme for initial value problems formulated by Ramos in [Applied Mathematics and Computation 189 (2007), 710-718]. Moreover, the present approach can be extended to construct A-stable and L-stable high-order explicit one-step methods for differential equations.

Finally, the theoretical findings and advantages of the developed numerical methods are supported and illustrated by a series of numerical experiments in which stiff problems are considered.

Keywords: Stiff problems, Second-order scheme, L-stable, Nonlinear methods, Nonstandard finite difference method, non-local approximation
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*Corresponding author
**Corresponding author
Email addresses: tuanhm14@fe.edu.vn; hmtuan01121990@gmail.com (Manh Tuan Hoang), ehrhardt@uni-wuppertal.de (Matthias Ehrhardt)

1. Introduction

We begin by considering general initial value problems (IVPs) of the following form

$$y' = f(t, y), \quad y(0) = y_0 \in \mathbb{R}, \quad t \in [0, T]. \tag{1}$$

It is assumed that $f(t, y)$ satisfies suitable conditions that ensure that (1) has a unique solution. It should be emphasized that it is very difficult, even impossible, to solve the IVP (1) exactly. In most real-world situations, it is almost inevitable to find approximate solutions. For this reason, numerical methods for differential equations have become one of the most fundamental and practically important research tasks [1, 3, 4].

It is well known that the effective solution of stiff problems requires numerical methods possessing exceptional stability properties, such as A-stability and L-stability [1, 3, 4]. However, the construction of such numerical methods is not a trivial task. It has been proved that explicit Runge-Kutta methods cannot be A-stable and L-stable because their stability regions are bounded. Meanwhile, implicit Runge-Kutta methods can be A-stable and L-stable, but they are not as convenient as explicit methods because the solution of systems of nonlinear equations is required [1, 3, 4]. In [14], Nevanlinna and Sipila state a nonexistence theorem for A-stable explicit methods, which states that there are no A-stable explicit methods in a general class of "linear" methods. This class contains many well-known one-step and multistep numerical methods, such as Runge-Kutta and linear multistep methods, predictor-corrector methods, cyclic multistep methods, and linear multistep methods with higher derivatives.

With the goal of efficiently constructing explicit numerical methods for unconventional problems such as stiff problems or singular IVPs, nonlinear methods have been designed and developed by many researchers (see e.g. [2, 6, 7, 8, 17, 18, 19, 20, 21]). In [19], van Niekerk proposed a one-step first-order nonlinear method for IVPs based on a representation of the solution by the inverse of a polynomial. Then, in [17], Ramos further developed the ideas of [19] to construct an explicit nonstandard integration method for the IVP (1) in the form:

$$y_{n+1} = y_n + \frac{2hf_n^2}{2f_n - hf_n'}, \tag{2}$$

where $y_n = y(t_n)$, $y_{n+1} \approx y(t_{n+1})$, $f_n = f(t_n, y_n)$, $h = T/N$ ($N \in \mathbb{N}_+$) denotes the step size of the uniform grid $\{t_n = nh \,|\, n = 0, 1, \ldots, N\}$ and

$$f'_n = \frac{\partial f}{\partial t}(t_n, y_n) + \frac{\partial f}{\partial y}(t_n, y_n).$$

It is assumed that $y, f \in \mathbb{R}$. In [17] it was proved that the numerical method (2) is of second order and A-stable with stability function $R(z) = \frac{2+z}{2-z}$. It is important to note that the nonlinear methods presented in [16, 18, 21] are only A-stable.

Motivated and inspired by the A-stable second-order explicit nonlinear method constructed in [17], we present in this paper a simple approach to construct a general class of L-stable second-order explicit one-step methods for IVPs of the form (1). These methods are nonlinear and derive from a novel approximation for the function f on the right-hand side, inspired by the nonstandard finite difference method proposed by Mickens [9, 10, 11, 12, 13]. More precisely, we use a novel nonlocal approximation with weights to discretize the function on the right-hand side, and then impose suitable conditions such that the proposed methods are not only explicit and L-stable, but also convergent of order two. An important consequence is that our methods are suitable and efficient to solve stiff problems. Moreover, they also generalize and improve the one-step nonlinear method (2).

The plan of this work is as follows: In Section 2, second-order L-stable explicit numerical methods are constructed and analyzed. Numerical examples are reported in section 3. Concluding remarks and some open problems are discussed in Section 4.

2. Second-order *L*-stable explicit numerical methods

In this section, second-order L-stable explicit numerical methods are constructed and analyzed. First, we discretize the first derivative in (1) by the standard finite difference forward formula

$$y'(t_n) \approx \frac{y_{n+1} - y_n}{h}. \tag{3}$$

Next, the right-hand side function is approximated as follows:

$$\begin{aligned} f\big(t_n, y(t_n)\big) &= f\big(t_n, y(t_n)\big) + \Big(-y(t_n)A\big(t_n, y(t_n)\big) + y(t_n)A\big(t_n, y(t_n)\big)\Big) \\ &\approx f(t_n, y_n) - \alpha y_n A(t_n, y_n) + \alpha y_{n+1} A(t_n, y_n) + \beta h B\big(t_n, y(t_n)\big), \end{aligned} \tag{4}$$

where $A(t,y)$ and $B(t,y)$ are functions to be determined later; $\alpha, \beta \in \mathbb{R}$ play a role as weights in the discretization of the zero function, namely 0 can be approximated by

$$0 = -y(t_n)A\big(t_n, y(t_n)\big) + y(t_n)A\big(t_n, y(t_n)\big) \approx -\alpha y_n A(t_n, y_n) + \alpha y_{n+1} A(t_n, y_n),$$

and

$$0 \approx \beta h B\big(t_n, y(t_n)\big).$$

Remark 1. *This approximation allows us to construct L-stable second order explicit methods. If $B = 0$ or $\beta = 0$, i.e., the term $\beta h B\big(t_n, y(t_n)$ does not occur, our methods cannot be L-stable.*

Following the Mickens method [9, 10, 11, 12, 13], the above approximations can be considered as nonlocal approximations of the zero function. The approximations (3) and (4) lead to the family of finite difference methods

$$\frac{y_{n+1} - y_n}{h} = f(t_n, y_n) - \alpha y_n A(t_n, y_n) + \alpha y_{n+1} A(t_n, y_n) + h\beta B(t_n, y_n). \quad (5)$$

The scheme (5) can be rewritten in the fully explicit form

$$y_{n+1} = \frac{y_n + hf_n - h\alpha y_n A_n}{1 - h\alpha A_n - h^2 \beta B_n} = y_n + \frac{hf_n + h^2 \beta y_n B_n}{1 - h\alpha A_n - h^2 \beta B_n}, \quad (6)$$

where

$$f_n := f(t_n, y_n), \quad A_n := A(t_n, y_n), \quad B_n := B(t_n, y_n).$$

Note that $1 - h\alpha A_n - h^2 \beta B_n \neq 0$ provided that h is sufficiently small.

Theorem 1. *The truncation error of the one-step method* (5) *is* $\mathcal{O}(h^3)$ *if and only if the following relation is satisfied*

$$2\beta B_n y_n + 2\alpha A_n f_n = \frac{\partial f}{\partial t}(t_n, y_n) + \frac{\partial f}{\partial y} f(t_n, y_n) := f'_n. \quad (7)$$

Proof. First, it follows from the Taylor expansion of the function $y(t)$ that

$$y(t_{n+1}) = y(t_n) + hf\big(t_n, y(t_n)\big) + \frac{h^2}{2} f'\big(t_n, y(t_n)\big) + \mathcal{O}(h^3). \quad (8)$$

Let us denote by $f_D(t, y, h)$ the right-hand side function of (6), that is,

$$f_D(t, y, h) = y + \frac{hf(t,y) + h^2 \beta B(t,y) y}{1 - h\alpha A(t,y) - h^2 \beta B(t,y)}.$$

Then, we have

$$f_D(t,y,0)=y,\quad \frac{\partial f_D}{\partial h}(t,y,0)=f(t,y),\quad \frac{\partial^2 f_D}{\partial h^2}=2\alpha A(t,y)f(t,y)+2\beta B(t,y)y,$$

and combining it with the Taylor's expansion, we obtain

$$\begin{aligned} y_{n+1}=f_d(t_n,y_n,h)&=y_n+hf(t_n,y_n)\\ &+\frac{h^2}{2}\Big(2\alpha A(t_n,y_n)f(t_n,y_n)+2\beta B(t_n,y_n)y_n\Big)+\mathcal{O}(h^3). \end{aligned} \tag{9}$$

Hence, we deduce from (8) and (9) that

$$y(t_{n+1})-y_{n+1}=\mathcal{O}(h^3)$$

if and only if (7) holds. This is desired conclusion, the proof is complete. □

Remark 2. *Since the one-step method* (11) *is consistent of order two, we can use the approaches in [1, 3, 4] to conclude that it is also convergent of order two.*

We now give conditions for the method (5) to be L-stable. First, we consider a special case of the method (6), namely when β does not appear ($\beta=0$). Then the condition (7) reduces to

$$A_n=\frac{f'_n}{2\alpha f_n}. \tag{10}$$

Consequently, the method (6) becomes the scheme of Ramos (2). Therefore, it is only A-stable (see [17]).

Let us assume that $\beta\neq 0$ and $\alpha\neq 0$. Then, it follows from (7) that

$$B_n=\frac{f'_n-2\alpha A_n f_n}{2\beta y_n}. \tag{11}$$

Next, thanks to (11), we represent the method (6) in the fully explicit form

$$y_{n+1}=\frac{2y_n^2+2hy_nf_n-2h\alpha y_n^2A_n}{2y_n-2h\alpha A_ny_n-h^2f'_n+2h^2\alpha A_nf_n}, \tag{12}$$

which is convergent of order two.

Since $A(t, y)$ is arbitrary, to obtain L-stable methods, we first choose

$$A(t, y) = f_y(t, y) = \frac{\partial f}{\partial y}(t, y). \tag{13}$$

Then, applying the method (12)-(13) to the Dahlquist's test equation $y' = \lambda y$ ($Re\lambda < 0$) yields

$$y_{n+1} = R(z)y_n, \quad z := \lambda h, \quad R(z) := \frac{2 + (2 - 2\alpha)z}{2 - 2\alpha z + (2\alpha - 1)z^2}. \tag{14}$$

Here, $R(z)$ is called the stability function of the method (12)-(13) (see [3]).

Theorem 2. *The following assertions are true*

(i) The method (12)-(13) *is A-stable if $\alpha \geq \frac{1}{2}$.*

(ii) $\lim_{z\to-\infty} R(z) = 0$ *if and only if $\alpha \neq \frac{1}{2}$.*

Proof. First, it is easy to prove that the inequality $|R(z)| \leq 1$ is equivalent to

$$(16a-8)(\operatorname{Re}\lambda)^2 + (2a-1)^2\left[(\operatorname{Re}\lambda)^4 + (\operatorname{Im}\lambda)^4\right] - 8\operatorname{Re}\lambda - 4a(2a-1)(Re\lambda)^3 + (4a-8a^2)(\operatorname{Re}\lambda)(\operatorname{Im}\lambda)^2 + 2(2a-1)^2(\operatorname{Re}\lambda)^2(\operatorname{Im}\lambda)^2 \geq 0. \tag{15}$$

Note that $16a - 8 \geq 0$, $4a(2a-1) \geq 0$ and $4a - 8a^2 \leq 0$ since $a \geq 1/2$. Consequently, the inequality (15) holds if $\operatorname{Re}\lambda \leq 0$, which implies that the stability region S satisfies

$$S := \{z \in \mathbb{C}|\, |R(z)| \leq 1\} \supset \mathbb{C}^- := \{z \in \mathbb{C}|\operatorname{Re}(z) \leq 0\}.$$

Consequently, the method (12)-(13) is A-stable.

The second part of this theorem results from the direct use of the formula for $R(z)$. Here we note that $\lim\limits_{z\to-\infty} R(z) = -1$ if $\alpha = 1/2$. This completes the proof. □

Combining Theorems 1 and 2, we obtain the following assertion.

Theorem 3. *The following nonlinear one-step method*

$$y_{n+1} = \frac{2y_n^2 + 2hy_nf_n - 2h\alpha y_n^2 f_{y,n}}{2y_n - 2h\alpha f_{y,n}y_n - h^2 f_n' + 2h^2\alpha f_{y,n}f_n}, \quad f_{y,n} := \frac{\partial f}{\partial y}(t_n, y_n) \tag{16}$$

is L-stable and convergent of order two if $\alpha > \frac{1}{2}$. And if $\alpha = \frac{1}{2}$, then it is convergent of order two, but only A-stable.

In the sequel we briefly summarize our findings:

(i) The stability function $R(z)$ given in (14) differs from the ones of implicit Runge-Kutta methods presented in [1, 4]. In particular, when $\alpha = 1$, (16) reduces to

$$y_{n+1} = \frac{2y_n^2 + 2hy_nf_n - 2hy_n^2f_{y,n}}{2y_n - 2hf_{y,n}y_n - h^2f_n' + 2h^2f_{y,n}f_n}.$$

Its stability function $R(z)$ is given by

$$R(z) = \frac{1}{1 - z + z^2/2}.$$

The stability region in this case is sketched in Figure 1. It is clear that the stability region contains the left half complex plane. Consequently, the L-stability is confirmed.

(ii) The method (2) can be obtained from the method (5); thus, it is just a special case of (5). However, the approach used to construct (5) is different from that used to construct (2). The derivation of (5) is explained using nonlocal approximations for differential equations.

(iii) The nonlocal approximations of the zero function given in (4) extend the parameter space of the method (5). This is an important and crucial point in the construction of L-stable second order explicit methods. This strategy was used in our recent work [5] and can be extended to construct L-stable higher order explicit methods.

(iv) The method (16) can be applied to IVPs associated with systems of differential equations using component-wise implementations.

(v) Although the method (16) is only convergent of order two, it is simpler than an L-stable third-order explicit one-step method presented by Qureshi and Ramos in [15]. On the other hand, it is easy to improve its accuracy by variable step strategies or extrapolation techniques.

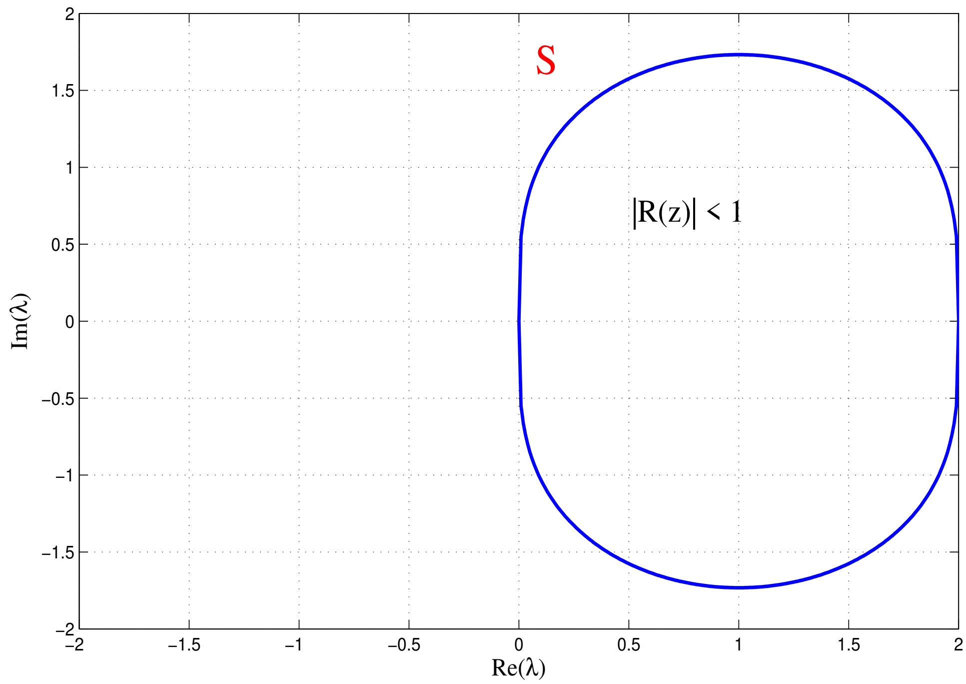

Figure 1: The stability region S of the method (12)-(13) when $\alpha = 1$, which is the part outside the blue curve ($|R(z)| = 1$).

3. Numerical experiments

In this section, we perform some illustrative numerical experiments to support the theoretical analysis.

Example 1 (The decay equation)**.** *Let us consider the well-known decay equation of the following form as a test problem.*

$$y' = \lambda y, \quad \lambda < 0, \quad y(0) = 1. \tag{17}$$

Its exact solution is given by $y(t) = e^{\lambda t}$. The larger $|\lambda|$ is, the faster y decreases.

We now apply the new L-stable second-order nonlinear explicit methods (16) (LENM2) with $\alpha = 0.55$ and the A-stable second-order explicit nonlinear method (2) (AENM2) to solve the decay equation (17), and then enter their absolute errors in Table 1. In this table, err_{end} and err_{max} are the absolute errors at the end of the time interval ($T = 1$) and the maximum of the absolute errors calculated at all grid points $t_n \in [0, 1]$, $n = 0, 1, \ldots, N$, respectively.

Table 1: Absolute errors for $y' = -2023y$, $y(0) = 1$, $t \in [0, 1]$.

h	LENM2 err_{max}	LENM2 err_{end}	AENM2 err_{max}	AENM2 err_{end}
0.5	0.0088	7.7131e-005	0.9961	0.9921
0.25	0.0173	9.0379e-008	0.9921	0.9689
0.2	0.0215	4.6304e-009	0.9902	0.9518
0.1	0.0417	1.5942e-014	0.9804	0.8206
0.05	0.0783	7.5965e-023	0.9612	0.4534
0.01	0.2487	3.6305e-061	0.8201	2.4250e-009
0.005	0.3042	4.0551e-104	0.6699	1.5596e-035

From the data presented in Table 1, it can be seen that the errors of the LENM2 scheme are better thanks to its L-stability.

Example 2 (A stiff problem). *Consider the following IVP*

$$y' = y^2 - e^{-2000t} - 1002e^{-1000t} - 1, \quad y(0) = 2. \tag{18}$$

The exact solution of (18) is given by $y(t) = e^{-1000t} + 1$. Thus, the solution drops very rapidly for a short time near 0 and then approaches the stable position $y^* = 1$. This is a typical feature of stiff problems. The errors obtained with the LENM2 with $\alpha = 0.6$ and the AENM2 are given in Table 2. It is clear that the LENM2 scheme gives better results.

Table 2: Absolute errors for (18) with $t \in [0, 0.1]$.

h	LENM2 err_{max}	LENM2 err_{end}	AENM2 err_{max}	AENM2 err_{end}
10^{-1}	0.9608	0.9608	0.9608	0.9608
10^{-2}	0.7471	0.7471	0.7475	0.7475
10^{-3}	0.0345	0.0097	0.0661	0.0661
10^{-4}	2.3750e-004	1.5534e-004	9.6796e-004	9.6796e-004
10^{-5}	2.2882e-006	1.6234e-006	1.0117e-005	1.0117e-005
10^{-6}	2.2797e-008	1.6307e-008	1.0163e-007	1.0163e-007
10^{-7}	2.2790e-010	1.4093e-010	1.0396e-009	1.0396e-009

Example 3 (A system of differential equations)**.** *Consider the following system of differential equations*

$$\begin{aligned} y_1' &= -1999y_1 - y_2^2, \quad y_1(0) = 1.0, \\ y_2' &= y_1 - y_2(1000 + y_2), \quad y_2(0) = 1.0. \end{aligned} \tag{19}$$

The exact solution is given by $(y_1(t), y_2(t)) = \left(e^{-2000t},\ e^{-1000t}\right)$. Thus, the equation (19) models a very stiff problem. The errors obtained with the LENM2 with $\alpha = 0.55$ and the AENM2 are given in the Tables 3 and 4. Similar to the Examples 1 and 2, the errors provided by the LENM2 scheme are better.

Table 3: Absolute errors generated by the LENM2 with $t \in [0, 0.1]$ in Example 3.

h	$\text{err}_{\max}(y_1)$	$\text{err}_{\text{end}}(y_1)$	$\text{err}_{\max}(y_2)$	$\text{err}_{\text{end}}(y_2)$
10^{-1}	0.0424	0.0424	0.0774	0.0774
10^{-2}	0.2511	9.5879e-007	0.3003	6.4413e-006
10^{-3}	0.0921	1.3839e-087	0.0239	3.7159e-044
10^{-4}	8.6724e-004	5.3884e-088	2.1422e-004	2.1147e-045
10^{-5}	8.6096e-006	6.7118e-090	2.1370e-006	2.1698e-047
10^{-6}	8.6061e-008	6.7248e-092	2.1366e-008	2.1700e-049

Table 4: Absolute errors provided by the AENM2 with $t \in [0, 0.1]$ in Example 3.

h	$\text{err}_{\max}(y_1)$	$\text{err}_{\text{end}}(y_1)$	$\text{err}_{\max}(y_2)$	$\text{err}_{\text{end}}(y_2)$
10^{-1}	0.9802	0.9802	0.9608	0.9608
10^{-2}	0.8182	0.1343	0.6667	0.0182
10^{-3}	0.1353	1.3839e-087	0.0345	3.7199e-044
10^{-4}	0.0012	6.9837e-088	3.0733e-004	2.9789e-045
10^{-5}	1.2265e-005	9.5519e-090	3.0705e-006	3.0990e-047
10^{-6}	1.2265e-007	9.5834e-092	3.0705e-008	3.1002e-049

4. Concluding remarks and open problems

In this work, we have proposed and analyzed a general class of L-stable explicit second-order one-step methods for solving stiff problems. The constructed methods are nonlinear and are derived from the novel approximation

(4) for the function f on the right-hand side of the IVPs, which is inspired by the nonstandard finite difference method introduced by Mickens. The main result is that we have obtained a general class of nonlinear one-step methods which are not only explicit and L-stable, but also convergent of order two. Therefore, they are suitable and efficient for solving stiff problems.

The proposed numerical methods generalize and improve the nonstandard explicit integration scheme (2) formulated by Ramos in [17]. Moreover, the present approach can be extended to construct high-order explicit one-step schemes that exhibit exceptional stability properties such as A-stable and L-stable.

Moreover, in Section 3 we have carried out a series of numerical experiments in which stiff problems are considered. As an important consequence, the advantages and superiority of the constructed methods are shown in all numerical examples considered.

Our future work will focus on applications of the constructed methods in solving differential equations arising in real situations. On the other hand, we intend to extend the findings and the present approach in this work to study the construction of explicit high-order one-step methods for stiff problems and singular problems.

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Authors' contributions:
M.T.H.: Conceptualization, Methodology, Software, Formal analysis, Writing-Original draft preparation
M.E.: Methodology, Analysis, Writing - Review & Editing, Supervision.
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