Global Journal of Science Frontier Research: F
Mathematics and Decision Sciences
Volume 24 Issue 2 Version 1.0 Year 2024
Type: Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Two Conservative Numerical Methods for Solving Initial Value Problems

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Abstract- According to the energy conservation equation, two novel conservative numerical methods are proposed for solving the second-order initial value problems. The C^1-continuous piecewise-quadratic functions are also used to approximate the true solutions. A priori error estimate is derived under a linear force assumption of the initial value problems. Some numerical tests are conducted to verify the theoretical results.

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GJSFR-F Classification: *MSC 2010: 65L20; 65L05; 65L70*

TWOCONSERVATIVENUMERICALMETHODSFORSOLVINGINITIALVALUEPROBLEMS

Two Conservative Numerical Methods for Solving Initial Value Problems

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Abstract- According to the energy conservation equation, two novel conservative numerical methods are proposed for solving the second-order initial value problems. The C^1-continuous piecewise-quadratic functions are also used to approximate the true solutions. A priori error estimate is derived under a linear force assumption of the initial value problems. Some numerical tests are conducted to verify the theoretical results.

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I. Introduction

As one of the most well-known natural laws, Newton's second law of motion can be expressed in the form of a second-order differential equation. In order to preserve the energy conservation property of the original system, it is very important to use the conservative numerical methods to solve these equations with initial conditions [1-4]. In recent years some conservative numerical methods [1-3] have been developed to solve the following second-order initial value problem,

$$\ddot{x}(t) = f\big(x(t)\big), t \in I;\ x(0) = \alpha;\ \ \dot{x}(0) = \beta, \tag{1.1}$$

where $I = (0, T)$, and $\dot{x} := \dfrac{\mathrm{d}x}{\mathrm{d}t}, \ddot{x} := \dfrac{\mathrm{d}^2x}{\mathrm{d}t^2}$.

Introduce the potential function $\phi(x)$ of $f(x)$,

$$-\frac{\mathrm{d}\phi}{\mathrm{d}x} = f(x),$$

then the energy conservation equation is derived as [1-2]

$$\frac{1}{2}\Big(\frac{\mathrm{d}x}{\mathrm{d}t}\Big)^2 + \phi(x) = \frac{1}{2}\beta^2 + \phi(\alpha). \tag{1.2}$$

Applying iterative computation, Greenspan [1] proposed two conservative implicit numerical methods to solve problem (1.1). According to the energy conservation equation (1.2), Qin [2] constructed an explicit energy-conserving method by using sign function, Sövegjártó [3] also developed conservative spline methods to solve this problem

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1. D. Greenspan, Conservative numerical methods for $\ddot{x} = f(x)$, *J. Comput. Phys.*, 56 (1984) 28-41.

numerically. In these methods [2-3], the function value at the current temporal node is numerically calculated first, and then the derivative value at the current temporal node is numerically computed, in which the sign function is used to prejudge the sign of the derivative value. We design an energy conservation method(numerical method I), which first calculates the derivative value and then calculates the function value, without using the sign function. Moreover, we use the C^1-continuous piecewise-quadratic functions [5-6] to approximate the true solution of problem (1.1), and construct a C^1-continuous energy conservation numerical method(numerical method II), these approximate solutions are global C^1-smooth on the entire temporal interval. Under a linear force assumption of the initial value problems, a priori error estimate for the numerical method II is deduced, which shows that the method has first-order convergence accuracy.

The remainder of the paper is organized as follows. In Section II and Section III, we propose two novel conservative numerical methods. We derive a priori error estimate for numerical method II in Section IV. The numerical experiments demonstrating the promising features of the conservative methods are displayed in Section V.

II. Numerical Method I

Let $0 = t_0 < t_1 < \cdots < t_N = T$ be a subdivision of $\bar{I}$. Define

$$I_n := (t_n, t_{n+1}),\ h := t_{n+1} - t_n,\ n = 0, \ldots, N-1,$$

denote the numerical solution x_n and v_n for $x(t_n)$ and $\dot{x}(t_n)$, respectively.
We construct the following numerical scheme satisfying (1.2) for problem (1.1).

$$v_{n+1} = v_n + hf(x_n),$$

$$\phi(x_{n+1}) = \frac{1}{2}\beta^2 + \phi(\alpha) - \frac{1}{2}(v_{n+1})^2. \tag{2.1}$$

From second equation of (2.1), x_{n+1} can be determined by Newton's method [7], where the initial guess $\tilde{x}_{n+1}$ of x_{n+1} is computed by the following equation,

$$\tilde{x}_{n+1} = x_n + hv_n + \frac{h^2}{2}f(x_n).$$

III. Numerical Method II

We apply the piecewise second-order polynomial $\varphi(t) \in C^1(\bar{I})$ to approximate the true solution $x(t)$ of problem (1.1). In each subinterval $I_n, n=0, \ldots, N-1,$ set

$$\varphi(t) = a_n^2(t-t_n)^2 + a_n^1(t-t_n) + \varphi_n, t \in I_n \tag{3.1}$$

with $\varphi_n := \varphi(t_n), \varphi_0 = \alpha,\ a_0^1 = \beta$. And the coefficients a_n^2 and $a_j^1(j = 1, \ldots, N-1)$ are yet to be computed. Noting the continuity condition $\varphi(t) \in C^1(\bar{I})$, we have

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7. A. Quarteroni; R. Sacco; F. Saleri, Numerical Mathematics, Springer, Berlin, 2000.

$$\varphi_{n+1} = a_n^2 h^2 + a_n^1 h + \varphi_n,$$

$$a_{n+1}^1 = 2a_n^2 h + a_n^1. \tag{3.2}$$

Inserting (3.2) into (1.2), we get

$$\frac{1}{2}(2a_n^2 h + a_n^1)^2 + \phi(a_n^2 h^2 + a_n^1 h + \varphi_n) = \frac{1}{2}\beta^2 + \phi(\alpha). \tag{3.3}$$

From (3.3), a_n^2 can be computed by Newton's method, where the initial guess $\tilde{a}_n^2$ of a_n^2 is determined by $\tilde{a}_n^2 = \frac{f(\varphi_n)}{2}$.

IV. Error Analysis

In this section, we assume $f(x) = -\lambda^2 x$ [8] and deduce the convergent result for numerical method (3.1)-(3.3).

On one hand, from (3.2) we have

$$\varphi_{n+1} - \varphi_n = \frac{h}{2}(a_{n+1}^1 + a_n^1), \tag{4.1}$$

and hence,

$$\begin{aligned} \varphi_{n+2} - 2\varphi_{n+1} + \varphi_n &= \frac{h}{2}(a_{n+2}^1 - a_n^1) \\ &= h^2\left(\frac{a_{n+2}^1 - a_{n+1}^1}{2h} + \frac{a_{n+1}^1 - a_n^1}{2h}\right) \\ &= h^2(a_{n+1}^2 + a_n^2). \end{aligned} \tag{4.2}$$

On the other hand, since $\phi(x) = \frac{\lambda^2 x^2}{2}$, applying (3.2), (4.1), and the energy conservation equation (1.2) we obtain

$$\begin{aligned} a_n^2 &= \frac{1}{2h}(a_{n+1}^1 - a_n^1) \\ &= \frac{1}{2h}\frac{(a_{n+1}^1)^2 - (a_n^1)^2}{a_{n+1}^1 + a_n^1} \\ &= \frac{1}{4}\frac{(a_{n+1}^1)^2 - (a_n^1)^2}{\varphi_{n+1} - \varphi_n} \end{aligned}$$

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8. G. A. Baker; V. A. Dougalis; S. M. Serbin, An approximation theorem for second-order evolution equations, *Numer. Math.*, 35 (1980) 127-142.

$$= -\frac{1}{2}\frac{\phi(\varphi_{n+1}) - \phi(\varphi_n)}{\varphi_{n+1} - \varphi_n}$$

$$= -\frac{\lambda^2}{4}(\varphi_{n+1} + \varphi_n)$$

$$= \frac{1}{4}(f_{n+1} + f_n). \tag{4.3}$$

Together with (4.2)-(4.3), this yields

$$\varphi_{n+2} - 2\varphi_{n+1} + \varphi_n = h^2(\frac{1}{4}f_{n+2} + \frac{2}{4}f_{n+1} + \frac{1}{4}f_n), n = 0, \ldots, N-2. \tag{4.4}$$

It is easy to conclude that method (4.4) is stable, of order 2 [9].
Furthermore, using (3.2) and (4.3) we have

$$\varphi_1 = a_0^2 h^2 + a_0^1 h + \varphi_0 = (-\frac{\lambda^2}{4}\varphi_1 - \frac{\lambda^2}{4}\alpha)h^2 + \beta h + \alpha\,,$$

i.e.,

$$\varphi_1 = \frac{4 - \lambda^2 h^2}{4 + \lambda^2 h^2}\alpha + \frac{4h}{4 + \lambda^2 h^2}\beta,$$

recall the Taylor's formula

$$x(h) = \alpha + \beta h + \frac{1}{2}\ddot{x}(\xi)h^2, 0 < \xi < h,$$

we get

$$x(h) - \varphi_1 = \frac{2\lambda^2 h^2}{4 + \lambda^2 h^2}\alpha + \frac{\lambda^2 h^3}{4 + \lambda^2 h^2}\beta + \frac{1}{2}\ddot{x}(\xi)h^2 = \mathcal{O}(h^2)\,,$$

which implies the starting values φ_0, φ_1 have second-order accuracy. Hence, by using Theorem 10.6 of chapter III in [9], we conclude that the convergent order of method (4.4) is 1. Thus, we obtain the following convergent theorem for numerical method II.

Theorem 4.1: Let $\varphi(t)$ and $x(t)$ be the functions given by (3.1) and (1.1), respectively. Assume that $f(x) = -\lambda^2 x$, then we have the following error estimates,

$$|\, x(t_i) - \varphi(t_i) \,| \leq Ch, i = 2, \ldots, N,$$

where C is a positive constant.

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9. E. Hairer; S. P. Nørsett; G. Wanner, Solving Ordinary Differential Equations I, second edition, Springer, Berlin, 1993.

V. Numerical Tests

Notes

We shall apply our two methods to solve three problems given in [1, 8] and display the error results.

Example 1 [1]. $\ddot{x} = x^2, t \in (0,1);\ x(0) = 1;\ \dot{x}(0) = 1.$

Example 2 [1]. $\ddot{x} = -\sin x, t \in (0,1);\ x(0) = \pi / 2;\ \dot{x}(0) = 0.$

In our numerical experiments, we use numerical method I to calculate Example 1 and Example 2. In Tables 1-2 we give the error results with different h, where Error:= $|x(1) - x_N|$. These results indicate that numerical method I is effective.

Table 1: Example 1:

Numerical results for numerical method I

h	Error
1/2	4. 31e−1
1/4	1. 76e−1
1/8	5. 79e−2
1/16	1. 66e−2

Example 3 [8]. $\ddot{x} = -100x, t \in (0,1);\ x(0) = 1;\ \dot{x}(0) = 0.$

We apply numerical method II to solve Example 3 with different h. The errors and the convergent order are displayed in Table 3, where Error:= $|x(1) - \varphi(1)|$. These results validate the conclusion in Theorem 4.1.

Table 2: Example 2:

Numerical results for numerical method I

h	Error
1/2	1.43e-2
1/4	4.32e-3
1/8	1.16e-3
1/16	3.01e-4

Table 3: Example 3:

Numerical results for numerical method II

h	Error	Convergent order
1/1000	2. 83e−1	---
1/2000	1. 39e−1	1. 03
1/4000	6. 87e−2	1. 02

Acknowledgment

This work was partially supported by the Principal's Foundation of Minjiang University (Project No. 103952020071) and by the Construction Project of Minjiang University (Project No. MJUSFJD2022013).

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