Applied Mathematics and Computation 320 (2018) 731–739

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Positivity preserving scheme based on exponential integrators

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ARTICLE INFO

MSC:
65L05
65P40
65L20

Keywords:
Positivity
Exponential integrators
Nonlinear differential equations
Numerical methods

ABSTRACT

Many phenomena in almost all areas of natural and engineering science are modelled by nonlinear differential equations. However, most of the explicit methods for time integration of nonlinear models fail to preserve some qualitative properties such as positivity of solutions. The major purpose of this study is to suggest a new explicit positivity preserving numerical method based on the exponential integrators. It is shown that the proposed method preserves the positivity of exact solution. Several examples are illustrated to confirm the theoretical result.

1. Introduction

Numerical schemes for nonlinear differential equations produce approximated results. However, it is expected for a numerical scheme to respect some qualitative properties of the exact solution. One of those important properties is preserving the nonnegativity of the solution. The related subjects for nonnegativity are positivity and maximum principle. These subjects are equivalent for the linear equations [17]. We refer the reader to the study [5] and references therein for the maximum principle. In [5] instead of using maximum principle preserving scheme, the authors proposed a method which cuts off the negative values in the computed solution at each time step and then continues the time integration with the corrected solution.

A great deal of effort has been spent for the positivity preserving of the differential equations. Mickens suggested a nonstandard finite difference scheme which preserves the positivity as well as the boundedness for differential equations in [6], for reaction-diffusion equation in [7], for Fisher's PDE (partial differential equation) having nonlinear diffusion term in [8].

Preserving positivity also plays important role in mathematical biology and in chemical processes since the quantities such as population or concentration should be naturally nonnegative. Thus, considerable researches can be found in the literature. For example, Mickens proposed in [9] the nonstandard scheme for a discrete model preserving the positivity for a coupled ordinary differential equation (ODE)'s modeling glycolysis which arises in living cells as a biochemical reaction, Dimitrov and Kojouharov studied on a positive and elementary stable nonstandard finite difference methods for prey–predator systems in [3], Arenas et al. developed a nonstandard numerical method in [1] for a SIRS (susceptible-infectious-recovered-susceptible) seasonal epidemiological model for RSV (Respiratory Syncytial Virus) transmission. In [16] the authors discussed procedures for nonnegative solutions of ODEs. They used some test problems which occur in chemistry and physics.

The novelty of this paper is to derive and analyze a new explicit numerical method preserving the positivity based on the exponential integrators. To provide the theoretical result we shall first introduce exponential integrators and the general

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https://doi.org/10.1016/j.amc.2017.10.027
0096-3003/

discussion on positivity condition. Section 2 is dedicated for these requirements. The brief outlines are followed by the proof of positivity of the proposed method. In Section 3, we use some test problems that occurs in chemistry, physics and mathematical biology to confirm our theoretical result. Finally, Section 4 involves conclusions and several remarks.

2. Useful definitions and analysis of the method

In this section, exponential integrators will be briefly introduced. Secondly, we give the positivity condition on any system of ODEs. Finally, we derive and analyse a positivity preserving exponential integrator.

Exponential integrators are derived from *variation-of-constant formula* for numerical treatment of stiff systems. For linear equation these integrators produce exact solution as Nonstandard Finite Difference [6] and Exponentially Fitted Finite Difference [12,13] do. In general for nonlinear equations, nonlinear terms are discretized to obtain efficient and stable explicit schemes. The overview of these integrators is given in [14]. We mainly consider exponential time differencing (ETD). Consider one-dimensional semi-linear initial value problem

$$x'(t) = cx + F(x), \quad x(0) = x_0 \tag{1}$$

where c is a constant and $F(x)$ is nonlinear forcing term. The *variation-of-constant formula* for this ODE is given by

$$x(t_{k+1}) = x(t_k)e^{c\Delta t} + e^{c\Delta t}\int_0^{\Delta t} e^{-c\tau}F(x(t_k+\tau))d\tau. \tag{2}$$

The approximation $F(x(t_k+\tau)) \approx F(x(t_k))$ and exact integration of the exponential term inside the integral yield

$$x_{k+1} = x_k e^{c\Delta t} + F(x_k)\frac{e^{c\Delta t}-1}{c} \tag{3}$$

The scheme (3) is called ETD1 in [2].

A general d-dimensional autonomous nonlinear evolutionary system of ODEs

$$\mathbf{x}'(t) = \mathbf{f}(\mathbf{x}(t)) \quad \mathbf{x}(0) = \mathbf{x}_0 \geq \mathbf{0}, \quad 0 \leq t \leq t_{end} \tag{4}$$

where $\mathbf{x}(t) \in \mathbb{R}^d$ and $\mathbf{f} : \mathbb{R}^d \to \mathbb{R}^d$.

Throughout the paper, the nonnegativity of a vector $\mathbf{x} \in \mathbb{R}^d$ is defined as nonnegativity of each component of that and denoted by $\mathbf{x} \geq \mathbf{0}$. To guarantee the positivity of the solution, we impose the following conditions

Assumption 1.

$$f^i(\mathbf{x}) \geq 0, \quad \forall \mathbf{x} \geq \mathbf{0} \quad \text{such that} \quad x^i = 0, \quad i = 1, \dots, d. \tag{5}$$

where f^i and x^i denote the ith components of the $\mathbf{f}$ and $\mathbf{x}$ respectively.

Due to this condition, vector field $\mathbf{f}$ pushes the trajectories back to positive domain whenever the solutions approach the boundary. For the detailed discussion we refer [4].

2.1. Derivation of the method

We, now, turn our attention to d-dimensional nonlinear system given in Eq. (4). By adding and subtracting $A\mathbf{x}(t)$ where $A \in \mathbb{R}^{d\times d}$ and by using *variation-of-constant formula* we have

$$\mathbf{x}(t_{k+1}) = e^{\Delta tA}\mathbf{x}(t_k) + \int_{t_k}^{t_{k+1}} e^{(t_{k+1}-s)A}(\mathbf{f}(\mathbf{x}(s)) - A\mathbf{x}(s))ds. \tag{6}$$

By following the lines in deriving ETD1 we have the following scheme, which is denoted by *PETD*1 for Eq. (4)

$$\mathbf{X}_{k+1} = \mathbf{X}_k + \varphi_1(\Delta tA)\mathbf{f}(\mathbf{X}_k)\Delta t. \tag{7}$$

where $\varphi_1(A) = \left(e^A - I\right)A^{-1}$ is a matrix valued function. It is easy to see *PETD*1 is a consistent scheme for any invertible matrix A. This provides us with flexibility to select a suitable A matrix. This matrix might be depend on $\mathbf{X}_k$ at each time level k. We prefer the notation $A_{\mathbf{x}_k}$ to emphasize this dependence.

2.2. Positivity preserving PETD1

Before writing the explicit expression $A_{\mathbf{x}_k}$ for d-dimensional system, let us discuss the following one-dimensional case

$$x'(t) = f(x(t)) \quad x(0) = x_0 \geq 0, \quad 0 \leq t \leq t_{end} \tag{8}$$

where $f : \mathbb{R} \to \mathbb{R}$. Assumption 1 implies $f(0) \geq 0$. The corresponding *PETD1* method becomes

$$x_{k+1} = x_k + \left(\frac{e^{\Delta t\alpha}-1}{\alpha}\right)f(x_k). \tag{9}$$