Available online at www.sciencedirect.com
ScienceDirect
Mathematics and Computers in Simulation 133 (2017) 337–350
MATHEMATICS AND COMPUTERS IN SIMULATION
www.elsevier.com/locate/matcom

Original articles

Universal approaches to approximate biological systems with nonstandard finite difference methods

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Received 2 October 2015; received in revised form 28 January 2016; accepted 14 April 2016
Available online 2 May 2016

Abstract

Nonstandard finite difference methods have been extensively used to numerically solve various problems in science and engineering. Most of those methods have been specifically designed to handle each problem separately and have been difficult to extend to other problems. In recent years, general nonstandard modeling approaches preserving key characteristics of autonomous dynamical systems have been proposed. In this paper, three of these numerical methods are presented and their performance is evaluated and compared in several different settings.

Keywords: Finite difference; Nonstandard; Elementary stable; Positivity; Dynamically consistent

1. Introduction

In the early 1980s, Potts considered "best" difference equation approximations to linear ordinary differential equations (ODEs) [33] and nonlinear ODEs such as the simple Duffing equation [32]. Based on Potts' observations, Mickens proved that given any ODE, there exists an exact difference equation which has zero local truncation error [22]. However, in order to construct an exact difference equation, in general, one needs the exact solution to the differential equation. Since the standard approach to constructing finite difference methods for solving differential equations can lead to incorrect behavior in the solutions (e.g. "ghost solutions", numerical instabilities and chaotic behavior [37]), Mickens, using the exact difference equations as a guide, proposed the modeling rules for constructing Nonstandard finite-difference (NSFD) methods as follows [22,23]:

Rule 1 *The orders of the discrete derivatives should be equal to the orders of the corresponding derivatives of the differential equation.*

Rule 2 *Denominator functions for the discrete derivatives, must, in general, be expressed in terms of more complicated functions of the step-sizes than those conventionally used.*

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http://dx.doi.org/10.1016/j.matcom.2016.04.007
0378-4754/

Rule 3 *Nonlinear terms should, in general, be replaced by nonlocal discrete representations.*

Rule 4 *Special conditions that hold for the solutions of the differential equations should also hold for the solutions of the finite difference scheme.*

Rule 5 *The scheme should not introduce extraneous or spurious solutions.*

Rule 6 *For differential equations having $N(\geqslant 3)$ terms, it is generally useful to construct finite difference schemes for various sub-equations composed of M terms, where $M < N$, and then combine all the schemes together in an overall consistent finite difference model.*

In 1994 [21], Mickens introduced the concept of *elementary stability*, the property which brings correspondence between the local stability at equilibria of the differential equation and the numerical method. In 2001, Anguelov and Lubuma [2] formalized some of the foundations which motivate Mickens' rules, including convergence properties of nonstandard schemes. They defined *qualitative stability* with respect to a given property, such as positivity of solutions, conservation laws, and stability of equilibria, to mean that a numerical method satisfies such a property for any time-step. In 2005, Mickens coined the term *dynamic consistency* [24], to mean that a numerical method is qualitatively stable with respect to all desired properties of the solutions to the differential equation. In 2011, Anguelov, Lubuma and Shillor [4], in an effort to expand the theory connecting continuous dynamical systems to discrete dynamical systems of numerical methods, introduced the concept of *topological dynamical consistency*, which expands even further the idea of dynamic consistency.

The main advantages of the NSFD methods are that they preserve some of the major dynamical properties of the approximated continuous system for any value of the discrete step-size. Such properties may include the positivity, boundedness, and monotonicity of solutions and the linear stability properties of the equilibria, among others. In addition, most of the NSFD methods have an explicit form, which makes them a computationally effective tool in the simulations of nonlinear dynamical systems.

Since the onset, many NSFD methods have been constructed for specific ODE and PDE systems used to model physical processes and chemical reactions along with biological interactions such as food-chain and epidemic models usually in 2–4 dimensions (e.g. [21,3,25,26,28,31,11,27,19,17,34,20,7,5,8,16,29,38]). The majority of these studies focus on preserving equilibria and their local stability as well as the positivity of the solutions which are among the critical properties of biological systems. Proposed numerical schemes are usually of first-order of accuracy and each scheme selects which terms from the right-hand side are discretized at the old and which at the new time and that is usually the key difference. However, most of these approaches are not easily generalizable to other systems of practical interest.

Between 2008 and 2015 two research groups suggested different nonstandard modeling approaches which provided universal ways to design NSFD methods for broad classes of dynamical systems. From 2005 to 2011, Dimitrov and Kojouharov designed NSFD methods that preserve positivity and elementary stability for a variety of special classes of autonomous dynamical systems [10–14] culminating with positive and elementary stable nonstandard (PESN) methods for general 2- and 3-dimensional productive–destructive systems (PDS). In 2015, this was extended to n-dimensional PDS by Dimitrov, Kojouharov and Wood [39]. Subsequently, based on similar discretization ideas, a new NSFD method for solving general autonomous systems with positive solutions was constructed by Kojouharov and Wood [40]. In 2014, Anguelov, Dumont, Lubuma and Shillor [1] used the NSFD methodology to construct a numerical method which is dynamically consistent for a large class of dynamical systems used in epidemiology. The NSFD method is elementary stable, and preserves several properties, including positivity of solutions, dissipativity, and global asymptotic stability of the disease free equilibrium.

In this paper, we summarize the aforementioned universal approaches and compare their performance for various step-sizes when applied to a specific four-dimensional HIV epidemic model. Among the metrics of interest are complexity, computational intensity and closeness to exact solutions, focusing on the latter here.

2. Definitions and preliminaries

Consider the n-dimensional dynamical system of the form

$$\frac{dx}{dt} = f(x); \quad x(0) \in \mathbb{R}^n_+, \tag{2.1}$$