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Efficient energy-preserving integrators for oscillatory Hamiltonian systems ☆

Xinyuan Wu *, Bin Wang, Wei Shi

Department of Mathematics, Nanjing University, Nanjing 210093, PR China
State Key Laboratory for Novel Software Technology, Nanjing University, Nanjing 210093, PR China

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ABSTRACT

In this paper, we focus our attention on deriving and analyzing an efficient energy-preserving formula for the system of nonlinear oscillatory or highly oscillatory second-order differential equations $q''(t) + Mq(t) = f(q(t))$, where M is a symmetric positive semi-definite matrix with $\|M\| \gg 1$ and $f(q) = -\nabla_q U(q)$ is the negative gradient of a real-valued function $U(q)$. This system is a Hamiltonian system with the Hamiltonian $H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T Mq + U(q)$. The energy-preserving formula exactly preserves the Hamiltonian. We analyze in detail the properties of the energy-preserving formula and propose new efficient energy-preserving integrators in the sense of numerical implementation. The convergence analysis of the fixed-point iteration is presented for the implicit integrators proposed in this paper. It is shown that the convergence of implicit Average Vector Field methods is dependent on $\|M\|$, whereas the convergence of the new energy-preserving integrators is independent of $\|M\|$. The Fermi–Pasta–Ulam problem and the sine–Gordon equation are carried out numerically to show the competence and efficiency of the novel integrators in comparison with the well-known Average Vector Field methods in the scientific literature.

1. Introduction

The recent growth of geometric numerical integration has resulted in the development of numerical solution of differential equations which systematically incorporate qualitative features of the original problem into their structure. It has been realized that a numerical method should be designed to preserve as much as possible the physical/geometric properties of the problem. We refer the reader to [20,34] for a good theoretical foundation of structure-preserving algorithms for ordinary differential equations. The behavior of first integrals under numerical integration has been discussed for a long time. Examples include automatic preservation of linear integrals by all Runge–Kutta methods, automatic preservation of quadratic integrals by some (the symplectic) Runge–Kutta (–Nyström) methods, some exponential integrators and some linearization-preserving integrators. We refer the reader to [36,10,8,21,30,27,26] for example on this subject. With this background, we pay attention to the numerical methods that preserve energy in Hamiltonian systems. For the Hamiltonian differential equations

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* Corresponding author at: Department of Mathematics, Nanjing University, Nanjing 210093, PR China.
E-mail addresses: xywu@nju.edu.cn (X. Wu), wangbinmaths@gmail.com (B. Wang), shuier628@163.com (W. Shi).

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$$q' = J^{-1}\nabla H(q), \tag{1}$$

where J is a skew-symmetric constant matrix and $\nabla H(q)$ is the gradient of the Hamiltonian $H(q)$, the Average Vector Field (AVF) formula is first written down in [29] and is defined as

$$q_{n+1} = q_n + h\int_0^1 J^{-1}\nabla H\big((1-\tau)q_n + \tau q_{n+1}\big)d\tau. \tag{2}$$

The authors in [11] showed the existence of energy-preserving B-series methods. The AVF formula is identified as an energy-preserving integrator and as a B-series method in [33]. The AVF formula exactly preserves the energy for an arbitrary Hamiltonian H and only needs evaluations of the vector field. Following [33], we refer the reader to [5,7,18,6] for more research work about the AVF formula. Another interesting class of energy-preserving integrators are "extended collocation methods" and "Hamiltonian boundary value methods", which exactly preserve energy of polynomial Hamiltonian systems (see, e.g., [3,23–25,4]).

In this paper, we are concerned with efficient energy-preserving integrators for the system of nonlinear oscillatory second-order differential equations of the form

$$\begin{cases} q''(t) + Mq(t) = f(q(t)), \quad t \in [t_0, T], \\ q(t_0) = q_0, \quad q'(t_0) = q_0', \end{cases} \tag{3}$$

where M is a $d \times d$ symmetric positive semi-definite matrix with $\|M\| \gg 1$ and $f : \mathbb{R}^d \to \mathbb{R}^d$ is the negative gradient of a real-valued function $U(q)$ and is a nonlinear mapping in general. In this paper $\|\cdot\|$ denotes the Euclidean norm. This kind of system usually arises in various fields of science and technology, such as applied mathematics, mechanics, physics, astronomy, molecular biology and engineering. As a typical example, when the method of lines is applied to wave equations, where spatial derivatives are approximated by appropriate finite difference formulas, this converts each partial differential equation (PDE) into a set of coupled oscillatory or highly oscillatory ordinary differential equations (ODEs) in time. Another typical example is the well-known Fermi–Pasta–Ulam problem [12], which is an important model of nonlinear classical and quantum systems of interacting particles in the physics of nonlinear phenomena. Obviously, the system (3) is simply the following initial value problem of oscillatory Hamiltonian system

$$\begin{cases} q' = \nabla_p H(p,q), \\ p' = -\nabla_q H(p,q), \\ q(t_0) = q_0, p(t_0) = p_0 \end{cases} \tag{4}$$

with the Hamiltonian (see [9])

$$H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T Mq + U(q). \tag{5}$$

We use the superscript T denote the transpose of a vector or a matrix throughout this paper.

In recent years there has been an enormous advance in dealing with the oscillatory system (3) and some useful approaches to constructing Runge–Kutta–Nyström (RKN) type methods have been proposed. We refer the reader to [16,15,22,19,14,37–39,46,48,44,28] for example. Very recently, the authors in [47] took account of the special structure of system (3) brought by the linear term Mq and formulated a standard form of the multidimensional ERKN methods (extended RKN methods). The ERKN methods perform numerically much better than the classical RKN methods due to taking advantage of the special structure of the equation brought by the linear term Mq. Then the symplecticity conditions for ERKN methods are investigated and presented in [45]. It is important to note that the symplecticity conditions for ERKN methods reduce to those for the classical RKN methods when $M = \mathbf{0}_{d\times d}$. It is known that the symplectic ERKN methods cannot exactly preserve the Hamiltonian of the system (4) in general.

If we apply the AVF formula (2) to the Hamiltonian system (4) or (3), then we have

$$\begin{aligned} q_{n+1} &= q_n + hp_n + \frac{h^2}{2}\int_0^1 g\big((1-\tau)q_n + \tau q_{n+1}\big)d\tau, \\ p_{n+1} &= p_n + h\int_0^1 g\big((1-\tau)q_n + \tau q_{n+1}\big)d\tau, \end{aligned} \tag{6}$$

where

$$g(q) = -Mq - \nabla_q U(q) = -Mq + f(q).$$

However, the AVF formula (6) for the Hamiltonian system (4) takes no account of the special structure brought by the linear term Mq of the system (4), or (3), equivalently. The energy-preserving numerical methods taking advantage of the special structure have not been well investigated so far. We notice that the linear term Mq now becomes a part of the integrand in the AVF formula (6) which makes the trouble in applications since the practical AVF methods are all implicit and the iterations are inevitable in general. In fact, the linear term Mq in AVF formula (6) will lead to the serious obstacle for the convergence of the fixed-point iteration. The snag with this linear term under the integral in the AVF formula (6) is that