Journal of Computational Mathematics
Vol.40, No.4, 2022, 573–591.

http://www.global-sci.org/jcm
doi:10.4208/jcm.2011-m2019-0272

A DISSIPATION-PRESERVING INTEGRATOR FOR DAMPED OSCILLATORY HAMILTONIAN SYSTEMS*

Wei Shi
College of Mathematical Sciences, Nanjing Tech University, Nanjing 211816, China
Email: shuier628@163.com
Kai Liu [1)]
School of Statistics and Data Science, Nanjing Audit University, Nanjing 210023, China
Email: laukai520@163.com

Abstract

In this paper, based on discrete gradient, a dissipation-preserving integrator for weakly dissipative perturbations of oscillatory Hamiltonian system is established. The solution of this system is a damped nonlinear oscillator. Basically, lots of nonlinear oscillatory mechanical systems including frictional forces lend themselves to this approach. The new integrator gives a discrete analogue of the dissipation property of the original system. Meanwhile, since the integrator is based on the variation-of-constants formula for oscillatory systems, it preserves the oscillatory structure of the system. Some properties of the new integrator are derived. The convergence is analyzed for the implicit iterations based on the discrete gradient integrator, and it turns out that the convergence of the implicit iterations based on the new integrator is independent of $\|M\|$, where M governs the main oscillation of the system and usually $\|M\| \gg 1$. This significant property shows that a larger stepsize can be chosen for the new schemes than that for the traditional discrete gradient integrators when applied to the oscillatory Hamiltonian system. Numerical experiments are carried out to show the effectiveness and efficiency of the new integrator in comparison with the traditional discrete gradient methods in the scientific literature.

Mathematics subject classification: 65L05, 65L07, 65L20, 65P10.
Key words: Weakly dissipative systems, Oscillatory systems, Structure-preserving algorithm, Discrete gradient integrator, Sine-Gordon equation, Continuous α-Fermi-Pasta-Ulam system.

1. Introduction

In the past few decades, much attention has been paid on geometric numerical integration. A numerical integration method is called geometric if it exactly preserves one or more physical/geometric properties such as first integrals, symplectic structure, symmetries and reversing symmetries, phase-space volume, Lyapunov functions, foliations etc. of the system. Geometric numerical methods have important applications in many fields, such as fluid dynamics, celestial mechanics, molecular dynamics, quantum physics, plasma physics, quantum mechanics, and meteorology. We refer the reader to [4, 5, 17, 22, 27, 34, 38] for recent surveys of this research.

* Received November 28, 2019 / Revised version received May 17, 2020 / Accepted November 23, 2020 / Published online April 13, 2021 /
1) Corresponding author

In this paper, we shall concentrate on the preservation of the dissipation for weakly dissipative perturbations of oscillatory Hamiltonian systems

$$\begin{cases} \dot{q} = \nabla_p H(p,q), \\ \dot{p} = -\nabla_q H(p,q) - \Gamma p, \\ q(t_0) = q_0, \quad p(t_0) = p_0 \end{cases} \tag{1.1}$$

with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^T p + \frac{1}{2}q^T M q + V(q), \tag{1.2}$$

where $q : \mathbb{R} \to \mathbb{R}^d$ represents generalized positions, $p : \mathbb{R} \to \mathbb{R}^d$ represents generalized momenta, $V : \mathbb{R}^d \to \mathbb{R}$ is the potential of the systems. M and $\Gamma \in \mathbb{R}^{d\times d}$ is symmetric and positive semi-definite. If the system has a major linear term and a comparably small nonlinear term, i.e., $\|M\| \gg \|\nabla_q V(q)\|$, the main oscillation of the system is governed by the matrix M [38]. The dissipation rate is governed by the matrix Γ [29].

Systems in form (1.1) arise in many applications, such as mechanics, astronomy, quantum physics, molecular biology and engineering, especially for models of Newtonian mechanics that include frictional forces. For example, in rolling bearing design, the objective is to minimize friction losses. System (1.1) can well describe the dynamics of such mechanical systems. It can be verified that the Hamiltonian of the system is dissipative at a rate relative to matrix Γ. More precisely, we have

$$\frac{d}{dt}H(p,q) = -p^T \Gamma p \leqslant 0. \tag{1.3}$$

The linear damping Γp considered here is the simplest example of Rayleigh damping. In numerical simulations, it is of importance to correctly approximate losses in energy at a dissipation rate as a function of Γ. This motivates a special study and analysis of dissipation-preserving integrators for the system. We say that a numerical integrator for (1.1) is dissipation-preserving if the integrator can give a numerical solution that owns a dissipation property analogue to (1.3), i.e.,

$$H(p_{n+1}, q_{n+1}) \leqslant H(p_n, q_n).$$

The idea of applying geometric integration schemes to weakly dissipative problems has been studied by many researchers. For instance, symplectic methods are superior to standard methods when applied to perturbed integrable systems (e.g. the Van der Pols equation), in the sense that weakly attractive invariant tori are much better preserved [17]. Energy-momentum schemes preserve the relative equilibria [1,2]. Variational methods applied to weakly dissipative systems show excellent numerical rate of energy dissipation compared to other methods [21]. Second-order conformal symplectic schemes for damped Hamiltonian systems are presented in [3]. There are also finite difference schemes preserving dissipative properties of PDEs [8].

System (1.1) exhibits an oscillatory property due to the quadratic term $\frac{1}{2}q^T Mq$ in $H(p,q)$, which would also be taken into account when designing the integrators. It is easy to see that (1.1) is simply the following oscillatory second-order differential equations

$$\begin{cases} \ddot{q}(t) + \Gamma\dot{q}(t) + Mq(t) = f(q(t)), \quad t \in [t_0, T], \\ q(t_0) = q_0, \quad \dot{q}(t_0) = p_0, \end{cases} \tag{1.4}$$

where $f : \mathbb{R}^d \to \mathbb{R}^d$ is the negative gradient of $V(q)$.