Applied Numerical Mathematics 170 (2021) 242–254

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

A dissipation-preserving scheme for damped oscillatory Hamiltonian systems based on splitting

Kai Liu [a], Ting Fu [a], Wei Shi [b,*]

[a] College of Applied Mathematics, Nanjing University of Finance & Economics, Nanjing 210023, PR China
[b] College of Mathematical Sciences, Nanjing Tech University, Nanjing 211816, PR China

ARTICLE INFO

Article history:
Received 2 July 2021
Accepted 1 August 2021
Available online 9 August 2021

Keywords:
Weakly dissipative Hamiltonian systems
Oscillatory systems
Structure-preserving algorithm
Discrete gradient
Sine-Gordon equation
Continuous Fermi-Pasta-Ulam system

ABSTRACT

In this paper, a new dissipation-preserving scheme is established for weakly dissipative perturbations of oscillatory Hamiltonian systems. The system exhibits a nonlinear oscillatory structure. The main oscillation is governed by a matrix M and the damping is governed by a matrix Γ. The new scheme preserves the oscillatory structure of the systems by incorporating the matrix M in the scheme based on the idea of ERKN methods. Meanwhile, the discrete gradient and splitting are used to construct the scheme such that the numerical solution possesses a nearly correct damping rate of the system. A main feature of the new scheme is that a relatively large stepsize can be chosen since the convergence of the implicit iterations in the scheme is shown to be independent of the matrices M and Γ. Three numerical experiments of perturbed Hamiltonian systems are conducted to show the effectiveness and the efficiency of the new scheme in comparison with the traditional discrete gradient methods.

1. Introduction

This paper focuses on the geometric numerical scheme for oscillatory Hamiltonian systems with weakly dissipative perturbations. A scheme is called geometric scheme if it could exactly retain some geometric and structural properties of the system such as symplectic structure, symmetries, first integrals, etc. For theoretical aspects concerning geometric numerical integration, the readers are referred to [15,24,34,40,1,4,20].

The present paper is devoted to proposing a dissipation-preserving scheme for damped oscillatory Hamiltonian systems

$$\begin{cases} \dot{q} = \nabla_p H(p,q) \\ \dot{p} = -\nabla_q H(p,q) - \Gamma p \\ q(t_0) = q_0,\ p(t_0) = p_0 \end{cases} \tag{1}$$

with the Hamiltonian

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

* Corresponding author.
E-mail address: shuier628@163.com (W. Shi).

https://doi.org/10.1016/j.apnum.2021.08.001
0168-9274/

where $q:\mathbb{R}\to\mathbb{R}^d$ and $p:\mathbb{R}\to\mathbb{R}^d$ are generalized coordinates, $V:\mathbb{R}^d\to\mathbb{R}$ is the potential of the systems. M and $\Gamma\in\mathbb{R}^{d\times d}$ are two symmetric and positive semidefinite matrices. System (1) exhibits an oscillatory property, which is mainly governed by the matrix M provided that the nonlinear term of the system is comparably small to the linear term, i.e., $||M||\gg||\nabla_q V(q)||$ [40]. The dissipation rate of the system is governed by the matrix Γ. More precisely, we have

$$\frac{d}{dt}H(p,q)=-p^T\Gamma p\leq 0. \tag{3}$$

Notice that if $\Gamma=0_{d\times d}$, system (1) is a Hamiltonian system without dissipation. The Hamiltonian $H(p,q)$ is invariant along the exact solution of the system.

Systems of the form (1) arise in many applications. For example, it can well describe the dynamics systems arising in rolling bearing design, the objective of the which is to minimize friction losses [27]. It also arises frequently from the spatial semi-discretizations of damped wave equations such as damped Klein-Gordon equations based on the method of lines [6].

While numerically simulating the system, it is meaningful to correctly approximate energy of the systems. This means that the scheme should preserve the Hamiltonian $H(p,q)$ as much as possible if $\Gamma=0_{d\times d}$, and give the (nearly) correct dissipation rate of the system. The energy preservation of the numerical schemes for Hamiltonian systems has been studied by many researches. Symplectic schemes are shown to nearly preserve the energy over exponentially long times in the stepsize [13]. The discrete gradient methods [11,19,30,32,26,31,8] and the Hamiltonian boundary value methods [5,18] have been developed in recent years which can preserve the energy of the system exactly. The geometric integration of dissipative problems also has been studied by many researchers. For instance, the weakly attractive invariant tori are preserved much better by symplectic methods in contrast to the standard methods when applied to perturbed integrable systems [15]; Geometric integration and conformal conservation laws for Hamiltonian partial differential equations with damping are studied in [28]; In [7], average vector field method is used to construct numerical schemes that preserve the energy for Hamiltonian partial differential equations.

It can be seen that system (1) is equivalent to the following oscillatory differential equations

$$\begin{cases}\ddot{q}(t)+\Gamma\dot{q}(t)+Mq(t)=f(q(t)), & t\in[t_0,T]\\ q(t_0)=q_0,\quad \dot{q}(t_0)=p_0,\end{cases} \tag{4}$$

where $f:\mathbb{R}^d\to\mathbb{R}^d$ is the negative gradient of $V(q)$. In the past decades, a variety of numerical methods for numerically solving the oscillatory systems with the form $\ddot{q}+Mq=g(q,\dot{q})$ has been developed. For example, Gautschi [10] proposed the Gautschi method based on trigonometric polynomials. Gautschi-type methods are constructed and analyzed by many researchers [17]. More useful techniques to devise Runge-Kutta-Nyström (RKN)-type schemes can be found in [14,12,9]. In [39], the extended Runge-Kutta-Nyström (ERKN) methods are formulated, where the main oscillatory term Mq is incorporated into the methods. The oscillatory structure of the system is captured much better by ERKN methods compared with the traditional RKN methods [35,38,41,37]. If $\Gamma=0_{d\times d}$, then (4) is an oscillatory Hamiltonian system without dissipation. In [21], an extended discrete gradient formula is constructed based on the discrete gradient and the ERKN method, which can preserve the oscillatory structure and the energy of the system simultaneously. However, it is not applicable for the case that the damping matrix $\Gamma\neq 0_{d\times d}$.

Inspired by the previous work, in this paper, based on the ERKN methods and splitting, we propose a dissipation-preserving scheme for the system (1) that can possess a discrete version of dissipation relation (3) while preserving the oscillatory structure. The structure of the paper is as follows. Some preliminaries on the discrete gradient method and splitting are introduced in Section 2. Section 3 is devoted to the derivation of the new dissipation-preserving scheme as well as the analysis of some properties of the new scheme. Three numerical experiments are given in Section 4 to show the efficiency and effectiveness of the new dissipation-preserving scheme. Finally, conclusions are given in the last section.

2. Preliminaries

2.1. Discrete gradient method

Assume that $H:\mathbb{R}^m\to\mathbb{R}$. The definition of a discrete gradient for H is given as follows. A discrete gradient for H is a continuous map $\overline{\nabla}H:\mathbb{R}^m\times\mathbb{R}^m\to\mathbb{R}^m$ satisfying

$$(z_1-z_0)^T\overline{\nabla}H(z_0,z_1)=H(z_1)-H(z_0)$$

for $\forall z_0,z_1\in\mathbb{R}^m, z_0\neq z_1$. For consistency in the continuous limit, one also requires

$$\overline{\nabla}H(z_0,z_0)=\nabla H(z_0).$$

A discrete gradient method for the system $z_t=K(z)\nabla H(z)$ with $K^T(z)=-K(z)$, is a map $z_0\mapsto z_1$ given by

$$\frac{z_1-z_0}{h}=\overline{K\nabla}H(z_0,z_1),$$

where $\overline{K}$ typically allowed to depend on z_0, z_1 and h, is some skew-symmetric matrix approximating the matrix $K(z)$ and $\overline{K}(0, z_0, z_0) = K(z_0)$ for consistency.

In the following, three examples of discrete gradient of $H(y)$ are given.

- The *mean value discrete gradient* (Harten et al. [16]):

$$\overline{\nabla}_1 H(z_0, z_1) := \int_0^1 \nabla H((1-\tau)z_0 + \tau z_1) d\tau, \quad z_0 \neq z_1. \tag{5}$$

- The *midpoint discrete gradient* (Gonzalez [11]):

$$\begin{aligned} \overline{\nabla}_2 H(z_0, z_1) :&= \nabla H(\frac{1}{2}(z_0 + z_1)) \\ &+ \frac{H(z_1) - H(z_0) - \nabla H(\frac{1}{2}(z_0 + z_1)) \cdot (z_1 - z_0)}{|z_1 - z_0|^2}(z_1 - z_0), \quad z_0 \neq z_1. \end{aligned} \tag{6}$$

  Both the mean value and the midpoint discrete gradient are second-order approximations to the value of the gradient at the midpoint $\frac{z_0 + z_1}{2}$. And they are both symmetric in sense that $\overline{\nabla}_i H(z_0, z_1) = \overline{\nabla}_i H(z_1, z_0), i = 1, 2$.

- The *coordinate increment discrete gradient* (Itoh and Abe [19]):

$$\overline{\nabla}_3 H(z_0, z_1) := \begin{pmatrix} \frac{H(z_1^1, z_0^2, z_0^3, \ldots, z_0^m) - H(z_0^1, z_0^2, z_0^3, \ldots, z_0^m)}{z_1^1 - z_0^1} \\ \frac{H(z_1^1, z_1^2, z_0^3, \ldots, z_0^m) - H(z_1^1, z_0^2, z_0^3, \ldots, z_0^m)}{z_1^2 - z_0^2} \\ \vdots \\ \frac{H(z_1^1, \ldots, z_1^{m-2}, z_1^{m-1}, z_0^m) - H(z_1^1, \ldots, z_1^{m-2}, z_0^{m-1}, z_0^m)}{z_1^{m-1} - z_0^{m-1}} \\ \frac{H(z_1^1, \ldots, z_1^{m-2}, z_1^{m-1}, z_1^m) - H(z_1^1, \ldots, z_1^{m-2}, z_1^{m-1}, z_0^m)}{z_1^m - z_0^m} \end{pmatrix}. \tag{7}$$

  Here z_i^j is the jth component of z_i and $0/0$ in the formula (7) is understood to be the partial derivative $\partial H / \partial z^i$. The coordinate increment discrete gradient $\overline{\nabla}_3 H$ is not symmetric. A symmetric version can be constructed by

$$\frac{1}{2}\left(\overline{\nabla}_3 H(z_0, z_1) + \overline{\nabla}_3 H(z_1, z_0)\right),$$

  which will also be a second-order approximation to $\nabla H(\frac{z_0 + z_1}{2})$.

System (1) can be reformulated into the following form

$$\dot{y} = J \nabla H(y) \tag{8}$$

where J is the $2d \times 2d$ constant matrix

$$J = \begin{pmatrix} 0 & I \\ -I & -\Gamma \end{pmatrix}$$

with I the $d \times d$ identity matrix. Applying the traditional discrete gradient method formally to the system (8) gives the scheme

$$\begin{cases} q_1 = q_0 + \dfrac{h}{2}(p_0 + p_1), \\ p_1 = p_0 - \dfrac{h}{2}\Gamma(p_0 + p_1) - h\left(\dfrac{1}{2}M(q_0 + q_1) + \overline{\nabla} H(q_0, q_1)\right). \end{cases} \tag{9}$$

One can verify that the scheme preserves the dissipation, since

$$\frac{H(p_1, q_1) - H(q_0, p_0)}{h} = -\left(\frac{p_0 + p_1}{2}\right)^T \Gamma \left(\frac{p_0 + p_1}{2}\right), \tag{10}$$

which is a discrete analogue for (3).

It is noticed that the scheme (10) has not taken full advantage of oscillatory structure brought by the term Mq. Moreover, since the scheme is implicit, the implicit iteration is required in each step, the convergence of which relies on the matrices M and Γ if the fixed-point iteration is applied. This places a very strict restriction on the choice of the stepsize. In this paper, we will address this issue based on ERKN methods and splitting.

2.2. Composition and splitting

Composition and splitting are two useful approaches to improving the order of a basic method while maintaining some desirable properties of the basic method [24,3,36]. Arbitrarily high-order numerical schemes are easily obtainable by composition.

Let χ_h be the basic method with low algebraic order but good structure-preserving properties and $\gamma_1, \ldots, \gamma_{s-1}, \gamma_s$ real numbers. Then the composition

$$\psi_h = \chi_{\gamma_s h} \circ \chi_{\gamma_{s-1} h} \circ \cdots \chi_{\gamma_1 h} \tag{11}$$

is called the corresponding composition method, where the coefficients γ_i are suitably chosen to ensure the high algebraic order of the approximation ψ_h. Meanwhile, the structure-preserving properties the basic method owns could still hold for the corresponding composition method. For example, the time-symmetry of the basic method χ_h will be inherited by the corresponding composition method ψ_h if the coefficients in (11) satisfy $\gamma_i = \gamma_{s+1-i}$ for $i = 1, 2, \ldots, s$.

The idea of splitting is that in the differential equation

$$\dot{x} = f(x), \quad x(0) = x_0 \in \mathbb{R}^m, \tag{12}$$

split the vector field $f(x)$ as $f(x) = f^{[1]}(x) + f^{[2]}(x) + \cdots + f^{[n]}(x)$ such that every subproblem

$$\dot{x} = f^{[i]}(x), \quad x(0) = x_0 \in \mathbb{R}^m, \quad i = 1, 2, \cdots, n \tag{13}$$

can be integrated exactly or easier to be treated numerically than the original system. Moreover, each subproblem may possess some structural features that are related to the original system, which can be solved by some geometric numerical integration schemes such that the inherited structures are preserved. If the flow $x(h) = \varphi_h^{[i]}(x_0)$ at $t = h$ to the ith subproblem is exact or at least first-order accurate numerically. Then the composition

$$\chi_h = \varphi_h^{[m]} \circ \cdots \circ \varphi_h^{[2]} \circ \varphi_h^{[1]} \tag{14}$$

gives an approximation of at least order one to the solution of the original system. Then taking (14) as the basic method and using the composition (11) will provide higher-order methods. One can also obtain higher-order splitting method in a similar way of composition, i.e., introduce additional coefficients a_{ij}, form the composition (14) with $\varphi_{a_{ij}h}^{[i]}$ and suitably determine the coefficients a_{ij} to increase the order of χ_h.

The splitting algorithm is widely used since it has the advantage of maintaining certain geometric characteristics of the system and due to its efficiency and simplicity. In [23], the authors considered a symmetric composition method based on the numerical integration of the ordinary differential equation $\dot{x} = X = A + B$, which requires the vector fields A and B to be fully integrable. A comprehensive description of the application of the splitting algorithm in the numerical ODEs is given in [25]. Splitting methods are presented for a certain class of time-dependent linear differential equations in [2]. Symplectic algorithms with minimum error in energy preservation are constructed for separable Hamiltonian systems based on splitting in [29].

3. The new dissipation-preserving scheme for system (4) based on splitting

Let us write system (1) as the following form

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \underbrace{\begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla V(q) \end{pmatrix}}_{f^{[1]}} + \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & -\Gamma \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix}}_{f^{[2]}}. \tag{15}$$

The corresponding two subproblems are given as

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla V(q) \end{pmatrix}, \begin{pmatrix} q(t_0) \\ p(t_0) \end{pmatrix} = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}. \tag{16}$$

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} 0 & 0 \\ 0 & -\Gamma \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q(t_0) \\ p(t_0) \end{pmatrix} = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}. \tag{17}$$

System (16) is an oscillatory Hamiltonian system with Hamiltonian (2) while system (17) is the dissipative part of the original system (1). From the variation-of-constants formula, the exact h-flow of the system (16) has the form

$$\begin{pmatrix} q(t_1) \\ p(t_1) \end{pmatrix} = \exp\left(h \begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}\right) \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} + \int_{t_0}^{t_1} \exp\left((t_1 - \xi) \begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}\right) \begin{pmatrix} 0 \\ -\nabla V(q(\xi)) \end{pmatrix} \mathrm{d}\xi, \tag{18}$$

where $h = t_1 - t_0$. Approximating $\nabla V(q(\xi))$ by its discrete gradient $\overline{\nabla} V(q_0, q_1)$ in the integral of the above equation yields the energy-preserving approximated h-flow for subproblem (16):

$$\begin{pmatrix} q_1 \\ p_1 \end{pmatrix} = \exp\left(h \begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}\right) \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} + \int_{t_0}^{t_1} \exp\left((t_1 - \xi) \begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}\right) \mathrm{d}\xi \begin{pmatrix} 0 \\ \overline{\nabla} V(q_0, q_1) \end{pmatrix}. \tag{19}$$

The approximated h-flow (19) is equivalent to the extended discrete gradient scheme [21]:

$$\varphi_h^{[1]} : \begin{cases} q_1 = \phi_0(K) q_0 + h\phi_1(K) p_0 - h^2 \phi_2(K) \overline{\nabla} U(q_0, q_1), \\ p_1 = -hM\phi_1(K) q_0 + \phi_0(K) p_0 - h\phi_1(K) \overline{\nabla} U(q_0, q_1), \end{cases} \tag{20}$$

where $K = h^2 M$ and the matrix-valued functions $\phi(K)$ are defined as [38]:

$$\phi_l(K) := \sum_{i=0}^{\infty} \frac{(-1)^i K^i}{(2i + l)!}, \quad l = 0, 1, \ldots. \tag{21}$$

Notice that the h-flow (20) preserves the Hamiltonian of the subproblem (16), i.e., $H(p_1, q_1) = H(p_0, q_0)$. On the other hand, the subproblem (17) can be solved exactly and the exact h-flow is given as

$$\varphi_h^{[2]} : \begin{cases} q_1 = q_0 \\ p_1 = e^{-\Gamma h} p_0. \end{cases} \tag{22}$$

Now consider the following composition method, referred as Strang splitting or Marchuk splitting method:

$$\varphi_h = \varphi_{h/2}^{[2]} \circ \varphi_h^{[1]} \circ \varphi_{h/2}^{[2]}.$$

More precisely, the method is given by the following procedure (half dissipation–preservation–half dissipation)

$$(q_0, p_0) \overset{\varphi_{h/2}^{[2]}}{\longmapsto} (q_{1/2}^1, p_{1/2}^1) \overset{\varphi_h^{[1]}}{\longmapsto} (q_{1/2}^2, p_{1/2}^2) \overset{\varphi_{h/2}^{[2]}}{\longmapsto} (q_1, p_1). \tag{23}$$

After some computation, the scheme admits the following one-step form:

$$\begin{cases} q_1 = \phi_0(K) q_0 + h\phi_1(K) e^{-\Gamma h/2} p_0 - h^2 \phi_2(K) \overline{\nabla} V(q_0, q_1), \\ p_1 = -e^{-\Gamma h/2} hM\phi_1(K) q_0 + e^{-\Gamma h/2} \phi_0(K) e^{-\Gamma h/2} p_0 - e^{-\Gamma h/2} h\phi_1(K) \overline{\nabla} V(q_0, q_1). \end{cases} \tag{24}$$

We have the following theorem on the dissipation preservation property of the new scheme (24).

Theorem 3.1. *The dissipation of the Hamiltonian (2) is preserved by the scheme (24) with the stepsize h, when applied to system (1), i.e.,*

$$H(p_1, q_1) \leqslant H(p_0, q_0).$$

Moreover, we have

$$H(p_1, q_1) - H(p_0, q_0) = \frac{1}{2} p_1^T (I - e^{\Gamma h}) p_1 + \frac{1}{2} p_0^T (e^{-\Gamma h} - I) p_0. \tag{25}$$

Proof. By considering the flow (23), one obtains that

$$\begin{cases} q_{1/2}^1 = q_0 \\ p_{1/2}^1 = e^{-\Gamma h/2} p_0 \end{cases} \quad \text{and} \quad \begin{cases} q_1 = q_{1/2}^2 \\ p_1 = e^{-\Gamma h/2} p_{1/2}^2. \end{cases} \tag{26}$$

Since the flow $\varphi_h^{[1]}$ is energy-preserving, we have

$$H(q_{1/2}^1, p_{1/2}^1) = H(q_{1/2}^2, p_{1/2}^2). \tag{27}$$

Combining (26) and (27) yields

$$H(q_0, e^{-\Gamma h/2} p_0) = H(q_1, e^{\Gamma h/2} p_1). \tag{28}$$

Therefore,

$$\frac{1}{2} p_0^T e^{-\Gamma h} p_0 + q_0^T M q_0 + V(q_0) = \frac{1}{2} p_1^T e^{\Gamma h} p_1 + q_0^T M q_1 + V(q_1).$$

Hence,

$$H(q_1, p_1) - H(q_0, p_0) = \frac{1}{2} p_1^T (I - e^{\Gamma h}) p_1 + \frac{1}{2} p_0^T (e^{-\Gamma h} - I) p_0.$$

Since the dissipative matrix Γ is symmetric and positive semidefinite, the eigenvalues of Γ satisfy $\lambda_\Gamma \geqslant 0$. Therefore the eigenvalues of matrices $I - e^{\Gamma h}$ and $e^{-\Gamma h} - I$ are nonpositive. Thus, both the matrices $I - e^{\Gamma h}$ and $e^{-\Gamma h} - I$ are also symmetric and negative semidefinite. This implies that $H(q_1, p_1) - H(q_0, p_0) \leqslant 0$. The proof is completed. □

Remark 3.1. If $\Gamma = 0_{d\times d}$, scheme (24) reduces to the extended discrete gradient scheme given in [21] for Hamiltonian system (16) without dissipation. Moreover, from (25), we have

$$\frac{H(p_1, q_1) - H(p_0, q_0)}{h} = \frac{1}{2} p_1^T \left(\frac{I - e^{\Gamma h}}{h} \right) p_1 + \frac{1}{2} p_0^T \left(\frac{e^{-\Gamma h} - I}{h} \right) p_0.$$

Taking the limit $h \to 0$ (then $q_1 \to q_0$ and $p_1 \to p_0$) on both sides of the equation yields

$$\lim_{h\to 0} \frac{H(q_1, p_1) - H(q_0, p_0)}{h} = -p_0^T \Gamma p_0.$$

Therefore, (25) can be viewed as a discrete analogue of the dissipation property (3) for the system (1).

The symmetry of a scheme plays an important role in the long-term simulation. The symmetry of a scheme is defined below (see [15]).

Definition 3.1. A method Φ_h with $\Phi_h^* = \Phi_h$ is called symmetric. Here, Φ_h^* is the adjoint method of the method Φ_h, defined as the inverse map of the original method with reversed time step $-h$, i.e., $\Phi_h^* := \Phi_{-h}^{-1}$.

The following theorem presents the symmetry of the scheme (24).

Theorem 3.2. *Assume that the discrete gradient $\overline{\nabla} V$ in (24) is symmetric in the sense that $\overline{\nabla} V(q_0, q_1) = \overline{\nabla} V(q_1, q_0)$ for all q_0 and q_1. Then the new scheme (24) (or equivalently (23)) is symmetric.*

Proof. A scheme is symmetric if exchanging $1 \leftrightarrow 0$, $h \leftrightarrow -h$ leaves the scheme unaltered. It is easy to verify that the flow $\varphi_h^{[2]}$ is symmetric. Meanwhile, the flow $\varphi_h^{[1]}$ is symmetric since $\overline{\nabla} V$ is symmetric by assumption [21]. Therefore, we have

$$\varphi_h^* = (\varphi_{h/2}^{[2]} \circ \varphi_h^{[1]} \circ \varphi_{h/2}^{[2]})^* = (\varphi_{h/2}^{[2]})^* \circ (\varphi_h^{[1]})^* \circ (\varphi_{h/2}^{[2]})^* = \varphi_{h/2}^{[2]} \circ \varphi_h^{[1]} \circ \varphi_{h/2}^{[2]} = \varphi_h.$$

The proof is completed. □

Corollary 3.1. *The scheme (24) is symmetric and of order two.*

Proof. By the fact the flow φ_h is at least first-order approximation to the exact solution and Theorem 3.2. □

In the following, we consider the computational issues of the scheme (24).

First of all, since the mean value discrete gradient has some good features such as automatic preservation of linear symmetries, linear covariance, linear symmetric reversibility, the discrete gradient $\overline{\nabla} H$ is chosen to be the mean value discrete gradient $\overline{\nabla}_1 H$ for the rest of the paper. Although it involves integrals that may not be evaluated explicitly. We can use quadrature formulas such as Gauss-Legendre quadrature formulas to approximate it effectively. The symmetry of the scheme can be inherited if the nodes of the quadrature formulas are chosen to be symmetric.

Secondly, the scheme (24) is implicit, therefore it requires to solve a system of nonlinear algebraic equations in every time step. The fixed-point iteration is used for the computation of the system, i.e.,

$$q_1^{k+1} = \phi_0(K) q_0 + \frac{h}{2} e^{-\Gamma h/2} \phi_1(K) p_0 - h^2 \phi_2(K) \int_0^1 \nabla V((1-\tau) q_0 + \tau q_1^k) d\tau, k = 0, 1, \ldots. \tag{29}$$

The convergence of the fixed-point iteration is analyzed in the following theorem.

Theorem 3.3. *Suppose that $\nabla V(q)$ satisfies a Lipschitz condition, with Lipschitz constant L, i.e.,*

$$\|\nabla V(q) - \nabla V(\tilde{q})\| \leqslant L\|q - \tilde{q}\|.$$

Then the iteration (29) in each time step is convergent provided

$$0 < h < \frac{2}{\sqrt{L}}.$$

Here $\|\cdot\|$ denotes the Euclidean vector/matrix norm.

Proof. Let

$$\Phi : q \to \phi_0(K)q_0 + \frac{h}{2}e^{-\Gamma h/2}\phi_1(K)p_0 - h^2\phi_2(K)\int_0^1 \nabla V((1-\tau)q_0 + \tau q)d\tau.$$

Then,

$$\|\Phi(q) - \Phi(\tilde{q})\| = \left\| h^2\phi_2(K)\left(\int_0^1 \nabla V((1-\tau)q_0 + \tau q) - \nabla V((1-\tau)q_n + \tau\tilde{q})d\tau\right)\right\|$$

Notice that the scalar functions $\phi_l(s), l = 0, 1, 2$ are bounded by $|\phi_l(s)| \leqslant \frac{1}{l!}, l = 0, 1, 2$, for $s \geqslant 0$. The matrix K is symmetric and positive semi-definite, hence it is orthogonally diagonalizable. Therefore, we have

$$\|\phi_l(K)\| \leqslant \frac{1}{l!}, l = 0, 1, 2.$$

Hence,

$$\|\Phi(q) - \Phi(\tilde{q})\| \leqslant \frac{h^2}{2}\left\|\int_0^1 \nabla V((1-\tau)q_0 + \tau q) - \nabla V((1-\tau)q_0 + \tau\tilde{q})d\tau\right\|$$

$$\leqslant \frac{h^2 L}{4}\|q - \tilde{q}\|.$$

Therefore, Φ is a contraction mapping by the assumption $0 < h < \frac{2}{L}$. The proof is completed. □

Remark 3.2. It is observed from Theorem 3.3 that the convergence of the iteration in every step of the scheme (24) is independent of the matrices M and Γ, which makes the choice of large stepsize possible. In comparison, if the subproblem (16) is solved by the traditional discrete gradient method, then though the resulting splitting scheme $\tilde{\varphi}_h$ has similar properties with the new scheme φ_h, it can be verified that the convergence of the iteration in every step of the scheme $\tilde{\varphi}_h$ will depend on the matrix M.

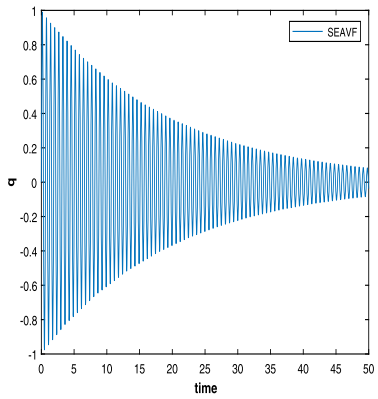
4. Numerical experiments

In order to show the accuracy and good behavior of dissipation preservation of the scheme (24) (denoted by SEAVF), three numerical experiments of perturbed Hamiltonian systems are conducted in this section. In the experiments, if the analytical solution of the problem is not available, the classical forth-order Runge-Kutta method in [15] with a sufficiently small stepsize is used to obtain the reference solution. We compare our scheme (24) with the scheme (9) (denoted by AVF) and the splitting scheme $\tilde{\varphi}_h$ mentioned in Remark 3.2 (denoted by SAVF). Same starting approximations are chosen for the implicit iterations of the three schemes in every step. The iteration will stop if $\|q_1^{k+1} - q_1^k\|$ is smaller than 10^{-15} or the number of iterations reaches 1000 in case that the iteration does not converge.

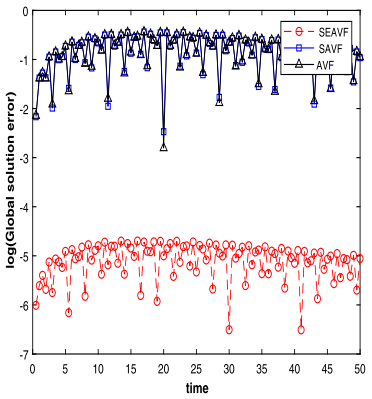
Problem 4.1. Consider the following damped Duffing equation

$$\begin{cases} \dot{q} = p \\ \dot{p} = -\omega^2 q + k^2(2q^3 - q) - \gamma p, t \in [0, t_{end}], \\ q(0) = 0, p(0) = \omega, \end{cases}$$

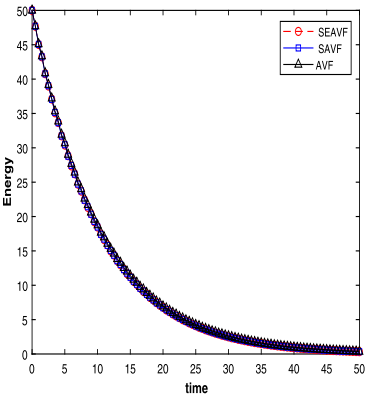
with Hamiltonian



(a) numerical solution by SEAVF

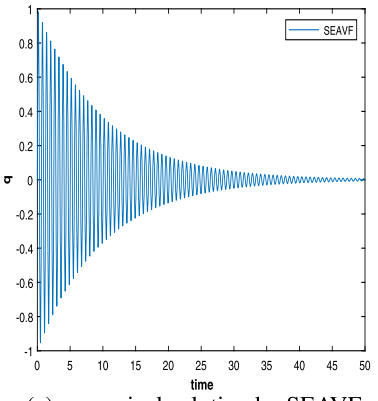


(b) global solution error

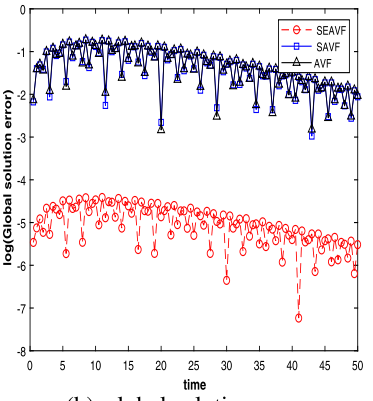


(c) energy decay

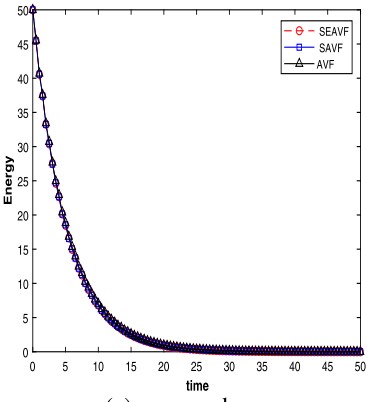
Fig. 1. Problem 4.1 with $\gamma = 0.1$.



(a) numerical solution by SEAVF



(b) global solution error



(c) energy decay

Fig. 2. Problem 4.1 with $\gamma = 0.2$.

Table 1
The CPU times and total number of iterations consumed by the three schemes in Problem 4.1.

		SEAVF	SAVF	AVF
$\gamma = 0.1$	CPU time (in seconds)	0.4163	1.2686	1.1195
	Total number of iterations	3996	28175	28754
$\gamma = 0.2$	CPU time (in seconds)	0.2277	0.9681	0.8819
	Total number of iterations	3987	27005	27830

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + V(q), \quad V(q) = \frac{k^2}{2}(q^2 - q^4),$$

coupled with $0 \le k < \omega$.

In this experiment, we set $\omega = 10, k = 0.03$. The equation is numerically integrated in the interval $[0, 50]$ for $\gamma = 0.1, 0.2$ with the stepsize $h = 1/40$. Fig. 1(a) and Fig. 2(a) present the numerical solutions given by SEAVF. The global solution errors of the three schemes are displayed in Fig. 1(b) and Fig. 2(b). As can be seen from Fig. 1(b) and Fig. 2(b), the scheme SEAVF gives the best approximation of the solutions among the three schemes. Fig. 1(c) and Fig. 2(c) show that all three schemes preserve the decay of the Hamiltonian at the same rate. In Table 1, we provide the CPU time and the total number of iterations consumed for every scheme to achieve the results. It is noted that though the three schemes are comparable for energy preservation, as expected, the numerical results still support that the scheme SEAVF is superior to the other two schemes concerning the accuracy and efficiency.

Problem 4.2. Consider the damped sine-Gordon equation with periodic boundary condition

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial^2 u}{\partial x^2} + \gamma \dfrac{\partial u}{\partial t} = -\sin u, \quad -L < x < L, t > 0, \\ u(-L, t) = u(L, t). \end{cases}$$

If $\gamma = 0$, the equation has the so-called breather-solution [33]

$$u(x,t) = 4\tan^{-1}\left(\frac{\sqrt{1-\omega^2}}{\omega}\frac{\cos\omega t}{\cosh(x\sqrt{1-\omega^2})}\right),$$

where $0 < \omega < 1$. The initial conditions are given by

$$u(x,0) = 4\tan^{-1}\left(\frac{\sqrt{1-\omega^2}}{\omega}\frac{1}{\cosh(x\sqrt{1-\omega^2})}\right),$$

and

$$u_t(x,0) = \frac{\partial}{\partial t}\left\{4\tan^{-1}\left(\frac{\sqrt{1-\omega^2}}{\omega}\frac{\cos\omega t}{\cosh(x\sqrt{1-\omega^2})}\right)\right\}_{t=0}.$$

Let $\Delta x = \frac{2L}{N}$ and $x_j = -L + j\Delta x$, $j = 0, \cdots, N$. Denote by $u_j(t)$ the numerical approximation of $u(x_j, t)$. If the spatial second-order derivative is approximated by the central finite difference

$$\delta^2 u_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2},$$

the damped sine-Gordon equation can be semi-discretized to a damped system of ODEs

$$\frac{d^2 u_j}{dt^2} + \gamma \frac{du_j}{dt} - \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} = -\sin u_j, \quad j = 1, \cdots, N, \tag{30}$$

where $u_0 = u_N$ and $u_{N+1} = u_1$.

By setting $q = (u_1, \cdots, u_N)$ and $p = \dot{q}$, the previous system (30) can be written in the following compact form

$$\begin{cases} \dot{q} = p \\ \dot{p} = -Mq - \nabla V(q) - \Gamma p, \quad t \in [0, t_{end}], \end{cases} \tag{31}$$

where $V(q) = (1 - \cos u_1) + \cdots + (1 - \cos u_N)$, $\Gamma = \gamma I$ and $M = -\dfrac{1}{\Delta x^2} D$ with

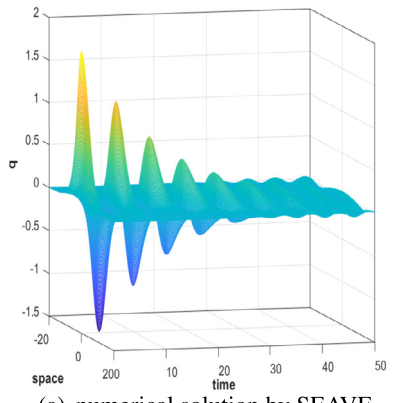
$$D = \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}.$$

In this experiment, we set $L = 20$, $\omega = 0.9$, $\gamma = 0.1$ and $N = 200$. The system (31) is numerically integrated in the interval $[0, 50]$ with stepsizes $h = 0.1$ and $h = 0.5$. The numerical results are shown in Fig. 3, Fig. 4 and Table 2. It is observed from the results that the three schemes with stepsize $h = 0.1$ have similar performance on the numerical accuracy and dissipation preservation. However, the new scheme SEAVF consumes the least CPU time and number of iterations among the three schemes. Furthermore, for the larger stepsize $h = 0.5$, the scheme SEAVF still gives a satisfactory result with even less CPU time consumption and number of iterations. Unfortunately, however, in this case, the schemes SAVF and AVF fail to give satisfactory numerical results since the iteration can not converge within 1000 steps.

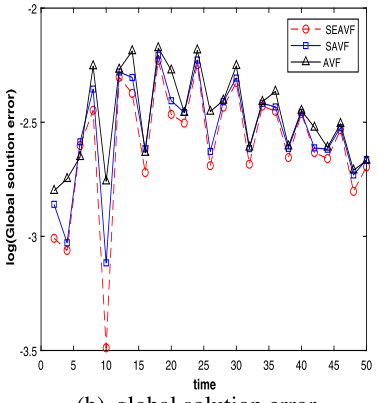
Problem 4.3. Consider a continuous generalization of $\alpha - FPU$ (Fermi-Pasta-Ulam) system (see, e.g. [22]) with homogeneous Dirichlet boundary condition

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} = \beta \dfrac{\partial^3 u}{\partial t \partial x^2} + \dfrac{\partial^2 u}{\partial x^2}\left(1 + \sigma\left(\dfrac{\partial u}{\partial x}\right)^k\right) - \gamma \dfrac{\partial u}{\partial t} - m^2 u, \quad 0 < x < L, t > 0, \\ u(0,t) = u(L,t) = 0, \end{cases} \tag{32}$$

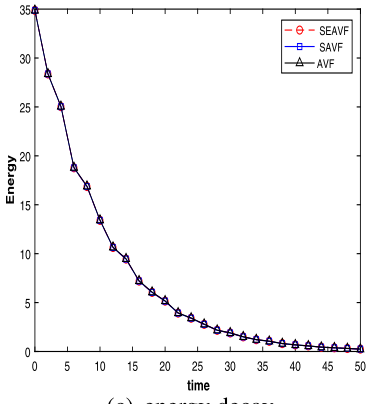
where $\sigma > 0, \beta, \gamma \geq 0$.



(a) numerical solution by SEAVF

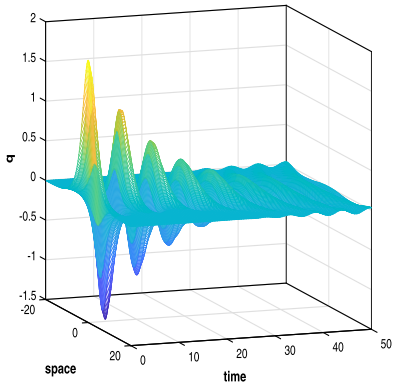


(b) global solution error

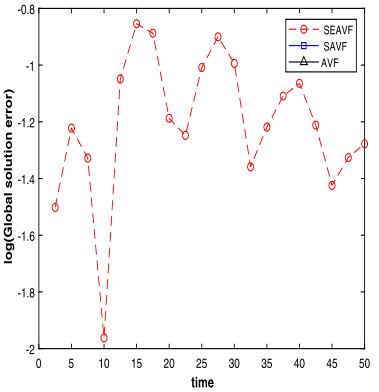


(c) energy decay

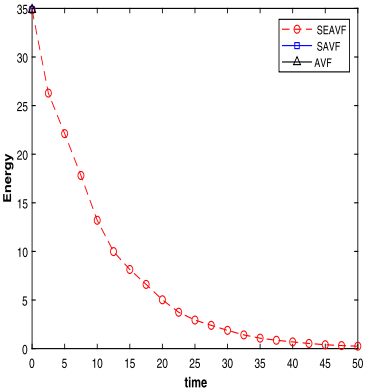
Fig. 3. Problem 4.2 with $h = 0.1$.



(a) numerical solution by SEAVF



(b) global solution error



(c) energy decay

Fig. 4. Problem 4.2 with $h = 0.5$.

Table 2
The CPU times and total number of iterations consumed by the three schemes in Problem 4.2.

		SEAVF	SAVF	AVF
$h = 0.1$	CPU time (in seconds)	6.2899	9.9571	16.3235
	Total number of iterations	3000	36036	76852
$h = 0.5$	CPU time (in seconds)	4.2927	NA	NA
	Total number of iterations	1292	NA	NA

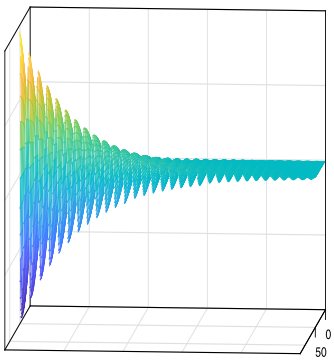
Let $\Delta x = \frac{L}{N}$, $x_j = j\Delta x$, $j = 0, \cdots, N$ and denote by $u_j(t)$ the numerical approximation of $u(x_j, t)$. If we discretize the second-order derivative in space with central finite differences and approximate the term $u_{xx}u_x^k$ by:

$$\frac{\partial^2 u}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^k|_{x=x_j} = \frac{1}{k+1}\partial_x\left(\frac{\partial u}{\partial x}\right)^{k+1}|_{x=x_j} \approx \frac{1}{k+1}\left(\left(\frac{u_{j+1}-u_j}{\Delta x}\right)^{k+1} - \left(\frac{u_j - u_{j-1}}{\Delta x}\right)^{k+1}\right)/\Delta x,$$

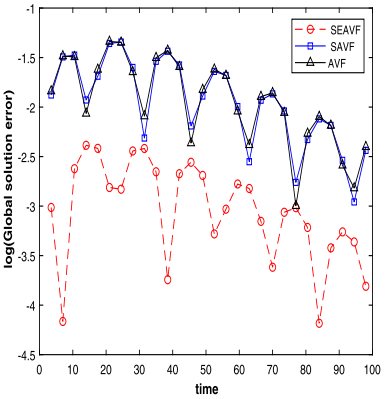
system (32) can be discretized as a damped system of ODEs

$$\begin{aligned}\frac{d^2u_j}{dt^2} - \frac{u_{j+1}-2u_j+u_{j-1}}{\Delta x^2} + m^2u_j - \frac{\beta}{\Delta x^2}\left(\frac{du_{j+1}}{dt} - 2\frac{du_j}{dt} + \frac{du_{j-1}}{dt}\right) + \gamma\frac{du_j}{dt} \\ = \frac{\sigma}{\Delta x^{k+2}}\frac{1}{k+1}\left((u_{j+1}-u_j)^{k+1} - (u_j - u_{j-1})^{k+1}\right), \quad j = 1, \cdots, N-1,\end{aligned} \tag{33}$$

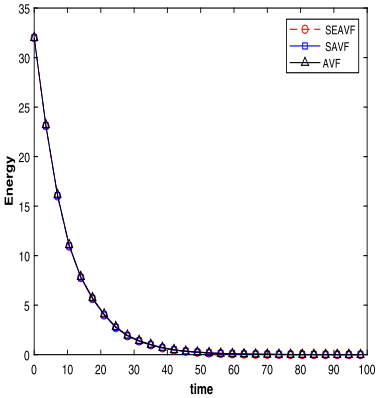
where $u_0(t) = u_N(t) = 0$.



(a) numerical solution by SEAVF



(b) global solution error



(c) energy decay

Fig. 5. Problem 4.3 with $\gamma = 0.1$, $\beta = 2$ and $h = 0.1$.

Table 3
The CPU times and total number of iterations consumed by the three schemes in Problem 4.3.

		SEAVF	SAVF	AVF
$h = 0.1$	CPU time (in seconds)	1.0073	3.1640	3.1612
	Total number of iterations	1233	11976	12221
$h = 0.5$	CPU time (in seconds)	0.2502	2.1412	2.1672
	Total number of iterations	308	9112	8867
$h = 1.0$	CPU time (in seconds)	0.1376	NA	NA
	Total number of iterations	156	NA	NA

System (33) can be written in compact form as in (31) with $M = m^2 I - \frac{1}{\Delta x^2} D$, $\Gamma = \gamma I - \frac{\beta}{\Delta x^2} D$ and

$$V(q) = \frac{\epsilon}{\Delta x^{k+2}} \frac{1}{(k+1)(k+2)} \sum_{j=0}^{N-1} (u_{j+1} - u_j)^{k+2},$$

by setting $q = (u_1, \cdots, u_{N-1})$ and $p = \dot{q}$. Here,

$$D = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}.$$

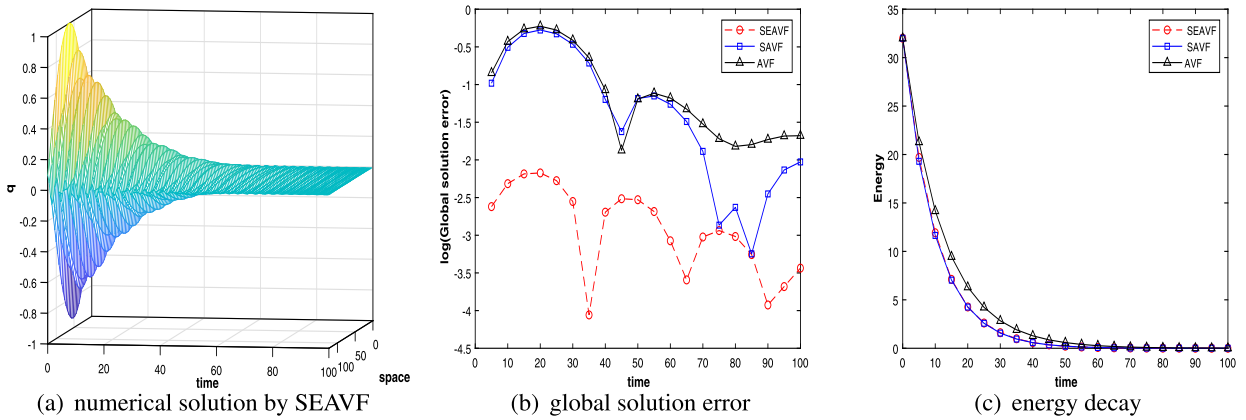
In this experiment, we set $k = 1, \sigma = \frac{3}{4}, m = 2, \gamma = 0.1$, $\beta = 2$ and $\Delta x = 1$. The associated initial conditions are:

$$u_n(0) = sin\left(\frac{n\pi}{N}\right), \quad \dot{u}_n(0) = 0, \quad n = 1, \cdots, N. \tag{34}$$

The mean value discrete gradients in the schemes are computed by the 2-point Gauss-Legendre quadrature:

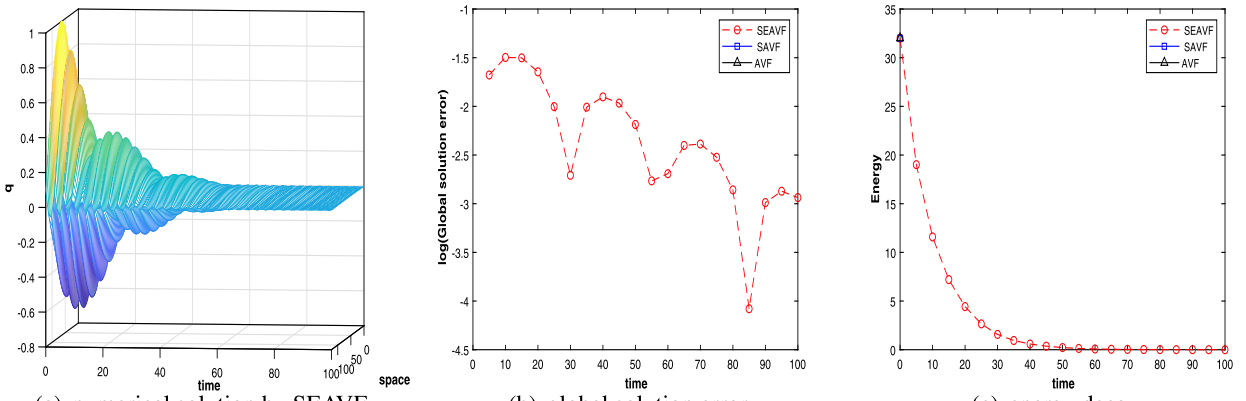
$$b_1 = \frac{1}{2}, b_2 = \frac{1}{2}, \quad c_1 = \frac{1}{2} - \frac{3^{\frac{1}{2}}}{6}, c_2 = \frac{1}{2} + \frac{3^{\frac{1}{2}}}{6}.$$

There is no quadrature error since the function $\nabla V(q)$ is a polynomial of degree two. The two parts γI and $\frac{\beta}{\Delta x^2} D$ contributes the damping of the system. The system is numerically integrated in the interval $[0, 100]$ with stepsizes $h = 0.1$, $h = 0.5$ and $h = 1.0$. The numerical results are shown in Fig. 5, Fig. 6, Fig. 7 and Table 3. It can be seen that with the same stepsize, the new scheme SEAVF behaves the best concerning the effectiveness and efficiency. The scheme SEAVF continues obtaining satisfactory numerical accuracy and energy preservation with less and less CPU time consumption and number of iterations as the stepsize h increases. On the contrary, the other two schemes fail when the stepsize h becomes large.



(a) numerical solution by SEAVF (b) global solution error (c) energy decay

Fig. 6. Problem 4.3 with $\gamma = 0.1$, $\beta = 2$ and $h = 0.5$.



(a) numerical solution by SEAVF (b) global solution error (c) energy decay

Fig. 7. Problem 4.3 with $\gamma = 0.1$, $\beta = 2$ and $h = 1.0$.

5. Conclusions

In this paper, numerical integration of the oscillatory Hamiltonian systems weakly perturbed by a linear damping is considered. Numerical schemes that can correctly approximate losses in energy at a dissipation rate closed to that of the system are preferred in numerical simulations. In this paper, a new dissipation-preserving scheme is derived based on discrete gradient and splitting. It can preserve a discrete version of the dissipation relation as well as the oscillatory structure of the original system. The convergence of implicit iteration is analyzed due to the implicity of the scheme. It is shown that a relatively large stepsize can be chosen since the convergence of the iteration only depends on the Lipschitz constant L of ∇V which is much smaller in comparison with $\|M\|$ and $\|\Gamma\|$. Therefore, the scheme is much favorable as long as the damped oscillatory Hamiltonian system is concerned. This has been confirmed in the numerical experiments. The efficiency and the effectiveness of the new scheme are also illustrated in the numerical results in comparison with the traditional discrete gradient methods.

Acknowledgement

The research was supported in part by the Natural Science Foundation of China under Grant 11701271.

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