

A LINEARLY-FITTED CONSERVATIVE (DISSIPATIVE) SCHEME FOR EFFICIENTLY SOLVING CONSERVATIVE (DISSIPATIVE) NONLINEAR WAVE PDES*

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Abstract

The extended discrete gradient method is an extension of traditional discrete gradient method, which is specially designed to solve oscillatory Hamiltonian systems efficiently while preserving their energy exactly. In this paper, based on the extended discrete gradient method, we present an efficient approach to devising novel schemes for numerically solving conservative (dissipative) nonlinear wave partial differential equations. The new scheme can preserve the energy exactly for conservative wave equations. With a minor remedy to the extended discrete gradient method, the new scheme is applicable to dissipative wave equations. Moreover, it can preserve the dissipation structure for the dissipative wave equation as well. Another important property of the new scheme is that it is linearly-fitted, which guarantees much fast convergence for the fixed-point iteration which is required by an energy-preserving integrator. The efficiency of the new scheme is demonstrated by some numerical examples.

Mathematics subject classification: 65L05, 65L07, 65L20, 65P10, 34C15.

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1. Introduction

Numerical schemes that conserve geometric structure have been shown to be useful when studying the long-time behaviour of dynamical systems. Such schemes are sometimes called geometric or structure-preserving integrators. The structure includes physical/geometric properties such as first integrals, symplecticity, symmetries and reversing symmetries, phase-space volume, Lyapunov functions, foliations. Geometric algorithms 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 [1–3] for recent

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surveys of this research. It has now become a common practice that the consideration of qualitative properties in ordinary and partial differential equations is important when designing numerical schemes. For ordinary differential equations (ODEs) it is possible to devise relatively general frameworks for structure preservation. This seems somewhat much more difficult for partial differential equations (PDEs) because PDEs are a huge and motley collection of problems and each equation under consideration normally requires a dedicated scheme (see, e.g. [6–10]). Fortunately, many attempts have been made to give a fairly general methodology to develop geometric schemes for PDEs. For example, in [4], by discretizing the energy of the PDEs to get an ODE system, then applying the average vector field method to the resulting system, the authors proposed a systematic procedure to deal with evolutionary PDEs as far as conservation or dissipation of energy is concerned. Another example is the PDEs that can be formulated into multi-symplectic form to which, one can apply a scheme which preserves a discrete version of this form (see, e.g. [5], for a review of this approach). Many energy-preserving or multi-symplectic methods are derived for Hamiltonian PDEs based on the multi-symplectic formulation (see, e.g., [11–14]).

In recent years, there has been an enormous advance in dealing with the oscillatory systems

$$\ddot{q} + Mq = f(q), \quad (1.1)$$

which can be obtained by spatial semi-discretization of wave equations and some useful approaches to constructing Runge-Kutta-Nyström (RKN)-type integrators have been proposed (see, e.g. [15–20]). Very recently, taking account of the special structure introduced by the linear term Mq , Wu *et al.* [20] formulated a standard form of the multidimensional extended RKN (ERKN) integrators. The ERKN integrators exhibit the correct qualitative behaviour much better than classical RKN methods due to using the special structure of the equation brought by the linear term Mq . For further work on this topic, we refer the reader to [19, 21, 22]. If f is the negative gradient of a scalar function V , i.e., $f = -\nabla V$, then (1.1) is a multi-frequency oscillatory Hamiltonian system. In [23], integrating the idea of the discrete gradient method with the ERKN integrator, the authors presented an extended discrete gradient formula for the oscillatory Hamiltonian system (1.1).

In this paper, we will propose and investigate an efficient approach to dealing with nonlinear wave PDEs following the line of [4]. Firstly, by approximating the functional whose negative variational derivative is the right-hand side term of the underlying wave equation, we semi-discretize the conservative wave equations into a Hamiltonian system of ODEs or the dissipative wave equations into a dissipative system of ODEs. We then apply the extended discrete gradient method to the resulting system of ODEs. This process gives a conservative scheme for conservative wave PDEs and a dissipative scheme for dissipative wave PDEs, and can be applied to a large scope of wave equations in a systematic way.

The outline of this paper is as follows. The preliminaries are given in Section 2. In Section 3, we recall the extended discrete gradient method, based on which a new dissipative scheme is proposed for dissipative systems with a damping term. In Section 4, the new numerical schemes are applied to some conservative/dissipative wave equations to show the efficiency and robustness in comparison with the existing methods in the literature. The last section focuses on some conclusions and discussions.

2. Preliminaries

We consider nonlinear wave PDEs of the form

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta \mathcal{G}}{\delta u}, \tag{2.1}$$

where

$$\mathcal{G}[u] = \int_{\Omega} G[u] dx, \quad \Omega \subseteq \mathbb{R}^d, \tag{2.2}$$

and $u : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^m$, $dx = dx_1 \cdots dx_d$. The square brackets in (2.2) indicate that a function depends on u itself as well as the derivatives of u with respect to the independent variables $x = (x_1, \dots, x_d)$ up to and including some degree ν . The variational derivative $\frac{\delta \mathcal{G}}{\delta u}$ is an m -vector, which can be defined through the relation

$$\int_{\Omega} \frac{\delta \mathcal{G}}{\delta u} \cdot v dx = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathcal{G}[u + \epsilon v], \tag{2.3}$$

for any sufficiently smooth m -vector of functions $v(x)$.

From now on, we assume that the solution has sufficient regularity and the boundary conditions on Ω are chosen such that the boundary terms vanish when calculating integration by parts (for example, periodic boundary conditions).

Take $d = 1$, $m = 1$ as an example. In this case, we have

$$\begin{aligned} \mathcal{G}[u] &= \int_{\Omega} G\left(u, \frac{\partial u}{\partial x}, \dots, \frac{\partial^{\nu} u}{\partial x^{\nu}}\right) dx, \\ \frac{\delta \mathcal{G}}{\delta u} &= \frac{\partial G}{\partial u} - \frac{\partial}{\partial x} \left(\frac{\partial G}{\partial u_x}\right) + \frac{\partial}{\partial x^2} \left(\frac{\partial G}{\partial u_{xx}}\right) + \dots + (-1)^{\nu} \frac{\partial}{\partial x^{\nu}} \left(\frac{\partial G}{\partial u^{(\nu)}}\right). \end{aligned}$$

For general m, d , the variational derivatives can be calculated by applying the Euler operator to $G[u]$ (see, e.g., [24] for details).

By our assumption, the equations of the form (2.1) have in common the energy conservation property

$$\frac{d}{dt} \mathcal{H}[u] = \frac{d}{dt} \int_{\Omega} \frac{1}{2} \left(\frac{\partial u}{\partial t}\right)^2 + G[u] dx = 0, \tag{2.4}$$

and usually we call it conservative. An important fact about wave PDEs (2.1) is that they can be represented as a system of first-order PDEs

$$\begin{pmatrix} u_t \\ w_t \end{pmatrix} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \tilde{\mathcal{H}}}{\delta u} \\ \frac{\delta \tilde{\mathcal{H}}}{\delta w} \end{pmatrix}, \tag{2.5}$$

where

$$\tilde{\mathcal{H}}[u, w] = \int_{\Omega} \frac{1}{2} w^2 + G[u] dx, \tag{2.6}$$

and $w = u_t$ is an intermediate function. Since

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

is skew-symmetric, based on the system representation (2.5), the conservation property is rewritten as the modified energy conservation property

$$\frac{d}{dt} \tilde{\mathcal{H}}[u, w] = 0. \tag{2.7}$$

In [4], by discretizing the energy functional $\tilde{\mathcal{H}}$ using a consistent approximation $\bar{H}\Delta x$, the authors semi-discretized the conservative PDEs (2.5) into a Hamiltonian system of ODEs with ‘skew-gradient’ form

$$\dot{y} = S\nabla\bar{H}(y), \quad y = \begin{pmatrix} U \\ W \end{pmatrix}, \tag{2.8}$$

where U and W denote the discrete values of u and $w = u_t$ at the mesh grid points.

Applying the discrete gradient method (see the next section) to the semi-discretized system yields the scheme

$$\frac{y_{n+1} - y_n}{\Delta t} = S\bar{\nabla}\bar{H}(y_n, y_{n+1}),$$

for advancing the numerical solution y_n at time t_n to y_{n+1} at time t_{n+1} , where $\bar{\nabla}\bar{H}(y_n, y_{n+1})$ is the discrete gradient of \bar{H} . The scheme preserves the discretized energy exactly.

Apart from the conservative case, we also consider the wave equations with a damping term

$$\frac{\partial^2 u}{\partial t^2} + \alpha \frac{\partial u}{\partial t} = -\frac{\delta \mathcal{G}}{\delta u}, \tag{2.9}$$

where $\alpha > 0$ is a small positive constant. The term αu_t represents a damping force proportional to the velocity u_t . Since the equations of the form (2.9) have in common the energy dissipation property

$$\frac{d}{dt} \mathcal{H}[u] = -\alpha \int_{\Omega} \left(\frac{\partial u}{\partial t} \right)^2 dx < 0, \tag{2.10}$$

we usually call it dissipative, i.e., $\mathcal{H}[u]$ is a Lyapunov function of (2.9). Wave equations (2.9) can be rewritten as

$$\begin{pmatrix} \dot{u}_t \\ \dot{w}_t \end{pmatrix} = \begin{pmatrix} 0 & I \\ -I & -\alpha I \end{pmatrix} \begin{pmatrix} \frac{\delta \tilde{\mathcal{H}}}{\delta u} \\ \frac{\delta \tilde{\mathcal{H}}}{\delta w} \end{pmatrix}, \tag{2.11}$$

and it is easy to verify that

$$D = \begin{pmatrix} 0 & I \\ -I & -\alpha I \end{pmatrix}$$

is semi-negative definite. Similar to the conservative case, semi-discretizing the dissipative PDEs (2.11) into a dissipative system of ODEs with the form

$$\dot{y} = D\nabla\bar{H}(y), \quad y = \begin{pmatrix} U \\ W \end{pmatrix} \tag{2.12}$$

and applying the discrete gradient method to system (2.12) gives the scheme

$$\frac{y_{n+1} - y_n}{\Delta t} = D\bar{\nabla}\bar{H}(y_n, y_{n+1}).$$

The scheme preserves the decay of the energy (see, e.g., [4]).

It is noted that in the case of the wave equations, in order to fit the framework in [4], we need to double the dimension of the systems which should be avoided from computational point of view. Furthermore, the wave equations have their own structures, which cannot be fully taken account of, if they are transformed into the form (2.5) or (2.11). For instance, the nonlinear Klein-Gordon equation can be written in the form (2.1):

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta \mathcal{G}}{\delta u}, \quad G[u] = \frac{u_x^2}{2} + \eta(u).$$

When using spatial semi-discretizations, a linear term naturally comes up due to the quadratic term $\frac{1}{2}u_x^2$ in $G[u]$. The special structure brought by the linear term could be considered when an efficient numerical scheme is designed. The extended discrete gradient method favors this point.

Based on the fact stated above, in this paper, instead of transforming the PDEs under consideration into the form (2.5), we consider directly the original form (2.1). Furthermore, we apply the extended discrete gradient method instead of the traditional discrete gradient method to the semi-discretized system of ODEs. More precisely, we first discretize the functional \mathcal{G} using some consistent approximation $\tilde{G}\Delta x$. The following lemma is useful and the proof can be found in [4].

Lemma 2.1. *Let*

$$\mathcal{H}[u] = \int_{\Omega} H[u] dx, \quad \Omega \subseteq \mathbb{R}^d, \quad (2.13)$$

and let $\bar{H}(U)\Delta x$ be any consistent (finite difference) approximation to $\mathcal{H}[u]$ (where $\Delta x = \Delta x_1 \cdots \Delta x_d$) with N degrees of freedom. Then in the finite-dimensional Hilbert space \mathbb{R}^N with the Euclidean inner product, the variational derivative $\frac{\delta}{\delta U}(\bar{H}(U)\Delta x)$ is given by $\nabla \bar{H}(U)$.

When approximating $\mathcal{H}[u]$ by a spectral discretization, despite that the approximation is not of the form in Lemma 2.1, the lemma still works since such an approximation can be viewed as a finite difference approximation where the finite difference stencil has the same number of entries as the number of grid points on which it is defined.

Let U represent the discrete values of u at the mesh grid points, in the multidimensional case after choosing an order. By Lemma 2.1, the variational derivative $\frac{\delta \mathcal{G}}{\delta u}$ is approximated by $\nabla \tilde{G}$. Thus, the wave equation (2.1) is semi-discretized into

$$\frac{d^2 U}{dt^2} = -\nabla \tilde{G}(U), \quad (2.14)$$

and the wave equation (2.9) with damping term is semi-discretized into

$$\frac{d^2 U}{dt^2} + \alpha \frac{dU}{dt} = -\nabla \tilde{G}(U). \quad (2.15)$$

We then apply the extended discrete gradient method to the systems (2.14) and (2.15), respectively. This process gives a conservative scheme for the conservative wave equations and a dissipative scheme for the dissipative wave equations. One of the benefits of using the extended discrete gradient method is that it is linearly-fitted which will be shown in the next section.

3. Extended Discrete Gradient Method

Discrete gradient methods for ODEs were introduced by Gonzalez [25], for research on discrete gradient methods, we refer the reader to [26–31].

We recall the definition of a discrete gradient. If $Q : \mathbb{R}^k \rightarrow \mathbb{R}$, the discrete gradient of Q is defined as follow.

Definition 3.1. *Let Q be a differentiable function. Then $\bar{\nabla}Q$ is a discrete gradient of Q provided it is continuous and for $\forall u, v \in \mathbb{R}^k, u \neq v$, satisfies*

$$\begin{cases} \bar{\nabla}Q(u, v) \cdot (u - v) = Q(u) - Q(v), \\ \bar{\nabla}Q(u, u) = \nabla Q(u). \end{cases} \tag{3.1}$$

Consider the continuous time systems of linear-gradient form:

$$\dot{y} = L(y)\nabla Q(y), \tag{3.2}$$

with $L(y)$ a matrix-valued function which is skew-symmetric for all y . Note that any ODE system preserving Q can be written in this form.

The corresponding discrete gradient method for (3.2) has the following form

$$\frac{y_{n+1} - y_n}{h} = \bar{L}(y_n, y_{n+1}, h)\bar{\nabla}Q(y_n, y_{n+1}), \tag{3.3}$$

where $\bar{L}(y_n, y_{n+1}, h)$ is some skew-symmetric matrix, which approximates the original $L(y)$. It is required that $\bar{L}(y, y, 0) = L(y)$ and $\bar{\nabla}Q(y, y) = \nabla Q(y)$ for consistency.

There are many possible choices of discrete gradients for a function Q (see, e.g. [25, 26, 32]), among which the one used in the average vector field (AVF) method is distinguished due to the fact that the AVF method has some good features such as linear covariance, automatic preservation of linear symmetries, reversibility with respect to linear reversing symmetries. Thus, from now on, we consider only the AVF method. The average vector field is defined as

$$\bar{\nabla}Q(y_n, y_{n+1}) := \int_0^1 \nabla Q((1 - \tau)y_n + \tau y_{n+1})d\tau. \tag{3.4}$$

A particular form of linear-gradient system (3.2) is the Hamiltonian system

$$\dot{y} = J^{-1}\nabla H(y), \tag{3.5}$$

with the Hamiltonian

$$H(p, q) = \frac{1}{2}p^\top p + \frac{1}{2}q^\top Mq + V(q), \tag{3.6}$$

where $y = (p^\top, q^\top)^\top$, $q = (q_1, q_2, \dots, q_N)^\top$, $p = (p_1, p_2, \dots, p_N)^\top$, $M \in \mathbb{R}^{N \times N}$ is a symmetric and positive semi-definite matrix. J is the $2N \times 2N$ skew-symmetric matrix

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

Applying the AVF method to the system (3.5) gives the scheme

$$\begin{cases} q_{n+1} = q_n + hp_n - \frac{h^2}{2} \left(\frac{1}{2}M(q_n + q_{n+1}) + \int_0^1 \nabla V((1 - \tau)q_n + \tau q_{n+1})d\tau \right), \\ p_{n+1} = p_n - h \left(\frac{1}{2}M(q_n + q_{n+1}) + \int_0^1 \nabla V((1 - \tau)q_n + \tau q_{n+1})d\tau \right). \end{cases} \tag{3.7}$$

It is easy to see that (3.5) is simply the following oscillatory second-order differential equations

$$\begin{cases} \ddot{q}(t) + Mq(t) = f(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, \quad \dot{q}(t_0) = p_0, \end{cases} \quad (3.8)$$

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

It is noted from Section 2 that the semi-discretized systems of many conservative wave equations can be formulated into the form (3.8) if all the linear terms with respect to U_i ($i = 1, \dots, N$) are attributed to MU .

Now, we are in a position to present the extended discrete gradient method for (3.8). Before doing that, we define the matrix-valued functions which appeared first in [19]

$$\phi_l(M) := \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+l)!}, \quad l = 0, 1, \dots \quad (3.9)$$

The extended discrete gradient formula is given in [23] for (3.8) as follows:

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\overline{\nabla}V(q_n, q_{n+1}), \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K)\overline{\nabla}V(q_n, q_{n+1}), \end{cases} \quad (3.10)$$

where h is the stepsize, $K = h^2M$, $p_n = \dot{q}_n$, and $\overline{\nabla}V(q_n, q_{n+1})$ is the discrete gradient of $V(q)$.

Remark 3.1. The matrix-valued functions $\phi_i, i = 0, 1, 2$ can be approximated by truncation of Taylor expansion. And Since the matrix-valued functions $\phi_i, i = 0, 1, 2$ only need to be calculated once for every fixed stepsize h , it does not add much extra computational cost on each iteration step. Based on the relationship among $\phi_i, i = 0, 1, 2$, other efficient algorithms for the computation of $\phi_i, i = 0, 1, 2$ can be found in [33] and the references therein.

Choosing $\overline{\nabla}V(q_n, q_{n+1})$ to be the average vector field gives the extended AVF method

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K) \int_0^1 \nabla V((1-\tau)q_n + \tau q_{n+1}) d\tau, \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K) \int_0^1 \nabla V((1-\tau)q_n + \tau q_{n+1}) d\tau. \end{cases} \quad (3.11)$$

It can be verified that the extended discrete gradient method is linearly-fitted in the sense that in the particular case where $\nabla V(q) \equiv \nabla V_0$ is constant, the extended discrete gradient method gives the exact solution of the system (3.5) or (3.8).

Moreover, note that all the schemes are implicit and require iterative computation, in general. A simple and common choice would be the fixed-point iteration. It is shown in [23] that the convergence of fixed-point iteration for the extended discrete gradient method is independent of $\|M\|$, however the traditional one does. This fact means that in general, a larger stepsize can be chosen for the extended discrete gradient schemes than that for the traditional discrete gradient methods. The convergence rate of fixed-point iteration for the extended discrete gradient method is higher than that for the traditional discrete gradient method.

The extended gradient methods can conserve the energy exactly when applied to the Hamiltonian system (2.14) (after reformulated into the form (3.8)). However, it cannot be applied

directly to the system of the form (2.15) because of the existence of the damping term. We now consider the following damped system

$$\begin{cases} \ddot{q}(t) + \alpha\dot{q}(t) + Mq(t) = f(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, \quad \dot{q}(t_0) = p_0. \end{cases} \tag{3.12}$$

We need to revise the extended gradient method so that it can be applied to (3.12). To this end, we put the term $\alpha\dot{q}$ to the right-hand side of the system and consider formally $\tilde{f}(q) = f(q) - \alpha\dot{q}$ as the negative gradient of the potential $\tilde{V}(q) = V(q) + \frac{\alpha}{2}\dot{q}^2$. System (3.12) is rewritten in the form

$$\begin{cases} \ddot{q}(t) + Mq(t) = \tilde{f}(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, \quad \dot{q}(t_0) = p_0. \end{cases} \tag{3.13}$$

Bearing in mind $p_n = \dot{q}_n$ and applying the extended discrete gradient method to (3.13) yields

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K) \left(\bar{\nabla}V(q_n, q_{n+1}) + \alpha\frac{p_n + p_{n+1}}{2} \right), \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K) \left(\bar{\nabla}V(q_n, q_{n+1}) + \alpha\frac{p_n + p_{n+1}}{2} \right). \end{cases} \tag{3.14}$$

The extended AVF method for (3.12) then becomes

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K) \left(\int_0^1 \nabla V((1-\tau)q_n + \tau q_{n+1})d\tau + \alpha\frac{p_n + p_{n+1}}{2} \right), \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K) \left(\int_0^1 \nabla V((1-\tau)q_n + \tau q_{n+1})d\tau + \alpha\frac{p_n + p_{n+1}}{2} \right). \end{cases} \tag{3.15}$$

All that remains is to prove that (3.14) preserves the dissipation or the decay of Lyapunov function $H(p, q)$. The following properties of matrix-valued functions play an important role in the proof:

$$\phi_0^2(K) + K\phi_1^2(K) = I, \quad K(\phi_1^2(K) - \phi_0(K)\phi_2(K)) = I - \phi_0(K), \tag{3.16a}$$

$$\phi_1^2(K) + K\phi_2^2(K) = 2\phi_2(K), \quad \phi_0(K) + K\phi_2(K) = I. \tag{3.16b}$$

Theorem 3.1. *If h is sufficiently small, the scheme (3.14) with the stepsize h preserves the dissipation or the decay of Lyapunov function $H(p, q)$ when applied to the damped system (3.12), i.e.,*

$$H(p_{n+1}, q_{n+1}) \leq H(p_n, q_n), \quad n = 0, 1, \dots$$

Proof. We first let

$$\bar{\nabla}\tilde{V}(q_n, q_{n+1}) = \bar{\nabla}V(q_n, q_{n+1}) + \alpha\frac{p_n + p_{n+1}}{2}.$$

Then compute

$$H(p_{n+1}, q_{n+1}) = \frac{1}{2}p_{n+1}^\top p_{n+1} + \frac{1}{2}q_{n+1}^\top Mq_{n+1} + V(q_{n+1}). \tag{3.17}$$

Using the symmetry of K and commutativity of K and all the $\phi_l(K)$ and inserting (3.14) into

(3.17), with a tedious computation we obtain

$$\begin{aligned}
 H(p_{n+1}, q_{n+1}) &= \frac{1}{2}p_n^\top (\phi_0^2(K) + K\phi_1^2(K))p_n + \frac{1}{2}q_n^\top M(\phi_0^2(K) + K\phi_1^2(K))q_n \\
 &\quad + q_n^\top K \left(\phi_1^2(K) - \phi_0(K)\phi_2(K) \right) \bar{\nabla} \tilde{V}(q_n, q_{n+1}) - hp_n^\top \left(\phi_0(K)\phi_1(K) \right. \\
 &\quad \left. + K\phi_1(K)\phi_2(K) \right) \bar{\nabla} \tilde{V}(q_n, q_{n+1}) + \frac{1}{2}h^2 \bar{\nabla} \tilde{V}(q_n, q_{n+1})^\top \left(\phi_1(K)^2 \right. \\
 &\quad \left. + K\phi_2(K)^2 \right) \bar{\nabla} \tilde{V}(q_n, q_{n+1}) + V(q_{n+1}). \tag{3.18}
 \end{aligned}$$

Substituting (3.16) into (3.18) gives

$$\begin{aligned}
 H(p_{n+1}, q_{n+1}) &= \frac{1}{2}p_n^\top p_n + \frac{1}{2}q_n^\top Mq_n + q_n^\top (I - \phi_0(K)) \bar{\nabla} \tilde{V}(q_n, q_{n+1}) \\
 &\quad - hp_n^\top \phi_1(K) \bar{\nabla} \tilde{V}(q_n, q_{n+1}) + h^2 \bar{\nabla} \tilde{V}(q_n, q_{n+1})^\top \phi_2(K) \bar{\nabla} \tilde{V}(q_n, q_{n+1}) + V(q_{n+1}) \\
 &= \frac{1}{2}p_n^\top p_n + \frac{1}{2}q_n^\top Mq_n + \left(q_n - (\phi_0(K)q_n + h\phi_1(K)p_n \right. \\
 &\quad \left. - h^2\phi_2(K) \bar{\nabla} \tilde{V}(q_n, q_{n+1})) \right)^\top \bar{\nabla} \tilde{V}(q_n, q_{n+1}) + U(q_{n+1}) \\
 &= \frac{1}{2}p_n^\top p_n + \frac{1}{2}q_n^\top Mq_n + (q_n - q_{n+1})^\top \bar{\nabla} \tilde{V}(q_n, q_{n+1}) + V(q_{n+1}) \\
 &= \frac{1}{2}p_n^\top p_n + \frac{1}{2}q_n^\top Mq_n + \alpha(q_n - q_{n+1})^\top \frac{p_n + p_{n+1}}{2} + V(q_n). \tag{3.19}
 \end{aligned}$$

The last equality is due to the definition of discrete gradient. Thus, we have

$$H(p_{n+1}, q_{n+1}) - H(p_n, q_n) = \alpha(q_n - q_{n+1})^\top \frac{p_n + p_{n+1}}{2}. \tag{3.20}$$

Solving the second equation of (3.14) for $\bar{\nabla} \tilde{V}(q_n, q_{n+1})$ and substituting it into the first equation of (3.14) yields

$$q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n + \phi_1^{-1}(K)\phi_2(K)(hp_{n+1} + K\phi_1(K)q_n - \phi_0(K)hp_n). \tag{3.21}$$

Substituting (3.21) into (3.20), we have

$$\begin{aligned}
 H(p_{n+1}, q_{n+1}) - H(p_n, q_n) &= -\alpha((\phi_0(K) - I)q_n + h\phi_1(K)p_n \\
 &\quad + \phi_1^{-1}(K)\phi_2(K)(hp_{n+1} + K\phi_1(K)q_n - \phi_0(K)hp_n))^\top \frac{p_n + p_{n+1}}{2} \\
 &= -2\alpha h \left(\frac{p_n + p_{n+1}}{2} \right)^\top \phi_1^{-1}(K)\phi_2(K) \frac{p_n + p_{n+1}}{2}. \tag{3.22}
 \end{aligned}$$

By the definition of matrix-valued functions and the assumption, it can be verified that $\phi_1^{-1}(K)\phi_2(K)$ is semi-positive definite. Thus, we have $H(p_{n+1}, q_{n+1}) - H(p_n, q_n) \leq 0$. The proof is complete. \square

Remark 3.2. If $M \rightarrow 0$, (3.14) reduces to the traditional discrete gradient method and (3.22) becomes

$$\frac{H(p_{n+1}, q_{n+1}) - H(p_n, q_n)}{h} = -\alpha \left(\frac{p_n + p_{n+1}}{2} \right)^\top \frac{p_n + p_{n+1}}{2}.$$

In this case, the scheme preserves the dissipation property regardless of the magnitude of the stepsize h . This coincides with the fact that discrete gradient methods are unconditionally energy-diminishing methods for dissipative gradient system (see [34]).

By now, we can give our scheme as follows.

- The scheme presented in this paper (denoted by EAVF):
 1. Discretize the functional $\mathcal{G}[u] = \int_{\Omega} G[u]dx$ using some consistent approximation $\bar{G}(U)\Delta x$ to get a system of ODEs ((2.14) or (2.15)) as described in the paper.
 2. The quadratic terms with respect to U in $\bar{G}(U)$ result in the linear terms $\nabla\bar{G}(U)$ of the semi-discretized system of ODEs. By attributing all these linear terms to MU , We can rewrite the system of ODEs in a form to which the extended AVF method is applicable.
 3. Apply the extended AVF method to the resulting system of ODEs.

Remark 3.3. By (3.20), we have

$$\frac{H(p_{n+1}, q_{n+1}) - H(p_n, q_n)}{h} = -\alpha \left(\frac{q_{n+1} - q_n}{h} \right)^T \frac{p_n + p_{n+1}}{2}. \tag{3.23}$$

Considering $(q_{n+1} - q_n)/h$ and $(p_n + p_{n+1})/2$ as two different approximations of $p_n = \dot{q}_n$, from this point of view, (3.23) is the discrete analogy of the dissipation property

$$\frac{d}{dt}\mathcal{H}[u] = -\alpha \int_{\Omega} \left(\frac{\partial u}{\partial t} \right)^2 dx.$$

Remark 3.4. If the damping coefficient α in (2.9) is space-dependent, i.e., $\alpha = \alpha(x)$ with the property $\alpha(x) > c$, where $c > 0$ is a positive constant, then it can be verified that (2.9) is still dissipative. To derive the corresponding linearly-fitted dissipative scheme, we only need to replace α in (3.14) by the diagonal matrix with diagonal entries being the discrete values of α at the mesh grid points. The preservation of dissipation can be proved in a similar way.

4. Numerical Experiments

In what follows, we apply the scheme presented in this paper to some conservative and dissipative wave equations to show the efficiency of the scheme. We compare the scheme derived in this paper with the scheme given in [4]. The scheme is described as follows.

- The scheme given in [4] (denoted by AVF):
 1. Discretize the energy functional

$$\mathcal{H}[u] = \int_{\Omega} \frac{1}{2} \left(\frac{\partial u}{\partial t} \right)^2 + G[u]dx$$

using some consistent approximation $\bar{H}(U)\Delta x$ to get a system of ODEs. Here, we choose

$$\bar{H}(U) = \sum_j \frac{1}{2} \dot{U}_j^2 + \bar{G}(U)$$

when comparing the two schemes. In this case, the resulting system of ODEs is the same as the one obtained by the scheme EAVF.

2. Then apply the traditional AVF method to the resulting system of ODEs.

All the computations and graphics are performed in MATLAB 7 in IEEE double precision arithmetic.

4.1. The AVF and starting approximations for fixed-point iteration

First, we consider the evaluation of the average vector field

$$\int_0^1 \nabla V((1 - \tau)q_n + \tau q_{n+1})d\tau.$$

For the system obtained by semi-discretizing PDEs, the potential $V(q)$ is typically of the form $V(q) = \sum_{i=1}^N a_i W(q^i)$, where W is a scalar function, q^i is the i th component of q and $a = (a_1, \dots, a_N) \in R^N$ is a constant vector (usually $a = (1, \dots, 1)^T$). The following lemma states that the average vector field can be evaluated exactly for this kind of special potential.

Lemma 4.1. *If $V(q) = \sum_{i=1}^N a_i W(q^i)$, then*

$$\int_0^1 \nabla V((1 - \tau)q_n + \tau q_{n+1})d\tau = \begin{pmatrix} a_1 \frac{W(q_{n+1}^1) - W(q_n^1)}{q_{n+1}^1 - q_n^1} \\ \vdots \\ a_i \frac{W(q_{n+1}^i) - W(q_n^i)}{q_{n+1}^i - q_n^i} \\ \vdots \\ a_N \frac{W(q_{n+1}^N) - W(q_n^N)}{q_{n+1}^N - q_n^N} \end{pmatrix}.$$

Proof. The proof is straightforward and we skip it. □

Since all the schemes derived in the paper are implicit, it is required to solve a system of nonlinear algebraic equations iteratively. A good starting approximation would improve the efficiency of the iteration. We refer the reader to [1] for details on the choice of good starting approximations for implicit schemes.

For conservative system, the unknowns q_{n+1} and p_{n+1} in the two schemes AVF and EAVF are decoupled. That means that we only need to solve q_{n+1} implicitly and p_{n+1} can be calculated explicitly. However, for dissipative system, the unknowns q_{n+1} and p_{n+1} are no longer decoupled, hence we have to solve them simultaneously by implicit iteration.

The most simple starting approximations for q_{n+1} and p_{n+1} are $q_{n+1} = q_n, p_{n+1} = p_n$ or $q_{n+1} = q_n + hp_n, p_{n+1} = p_n$. However, they are not accurate enough. Moreover, it is noted by Lemma 4.1 that the denominators in the evaluation of the integral are of the form $q_{n+1}^i - q_n^i$. We cannot choose the starting approximation $q_{n+1} = q_n$ or $q_{n+1} = q_n + hp_n$ if $p_n = 0$, since in this case, the implicit iteration will diverge immediately. Therefore, it is very subtle and takes much effort to give a proper starting approximation for the AVF method.

The scheme EAVF, however, gives us an idea to choose the starting approximations for q_{n+1} and p_{n+1} . Since the EAVF method integrates unperturbed systems exactly, we can choose

$$q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n, \quad p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n$$

as the starting approximations which is accurate enough. Moreover, we don't need extra calculation because they are exactly the part of the formulae of the scheme EAVF.

In order to compare the efficiency and convergence rate of the two schemes, we choose the same starting approximations for both schemes, i.e.,

$$q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n, \quad p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n.$$

4.2. Conservative wave equations

Problem 1. Consider the sine-Gordon equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \sin u, \quad t > 0.$$

We only consider the so-called breather-solution [35]

$$u(x, t) = 4 \tan^{-1} \left(\frac{\sqrt{1 - \omega^2}}{\omega} \frac{\cos \omega t}{\cosh(x\sqrt{1 - \omega^2})} \right). \tag{4.1}$$

The initial conditions are given by

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

with $\omega = 0.9$. On an infinite domain, this is a bump shaped solution which oscillates up and down with period $2\pi/\omega$. To exclude boundary effects, we use periodic boundary conditions with $L = 20$, i.e., we consider the sine-Gordon equation in the interval $[-20, 20]$.

The sine-Gordon equation is of the type (2.1) with

$$\mathcal{G}[u] = \int_{-L}^L \frac{1}{2} \left(\frac{\partial u}{\partial x} \right)^2 + (1 - \cos u) dx. \tag{4.2}$$

Denote $x_j = -L + j\Delta x$ with $\Delta x = \frac{2L}{N}$ and let

$$\bar{G}(U)\Delta x = \left(\sum_{j=0}^{N-1} \frac{1}{2(\Delta x)^2} (u_{j+1} - u_j)^2 + (1 - \cos(u_j)) \right) \Delta x$$

be the approximation of $\mathcal{G}[u]$. The resulting system of ODEs is given by

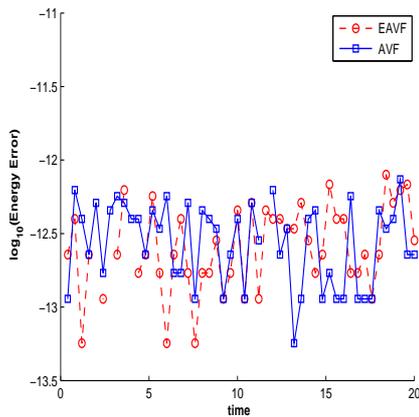
$$\frac{d^2 U}{dt^2} + MU = f(U), \tag{4.3}$$

where $U = (u_1, \dots, u_N)^T$, $f(U) = -\nabla V(U)$ with $V(U) = 1 - \cos(u_1) + \dots + 1 - \cos(u_N)$ and

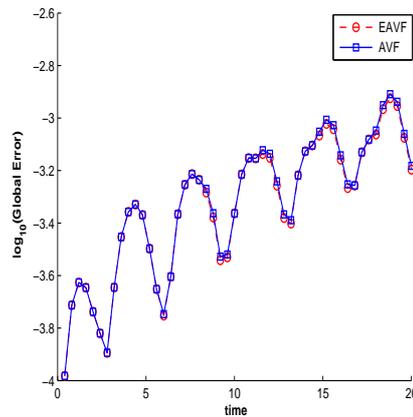
$$\begin{aligned} M &= \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}, \\ f(U) &= -\sin(U) = -(\sin u_1, \dots, \sin u_N)^T. \end{aligned}$$

Here, we use u_j to refer the value of u at x_j with a fixed time level.

The system is integrated in the interval $[0, 20]$ with $N = 400$ and $h = 0.01$. First, for the fixed-point iteration at each step, we set the error tolerance as 10^{-15} . We plot the logarithm

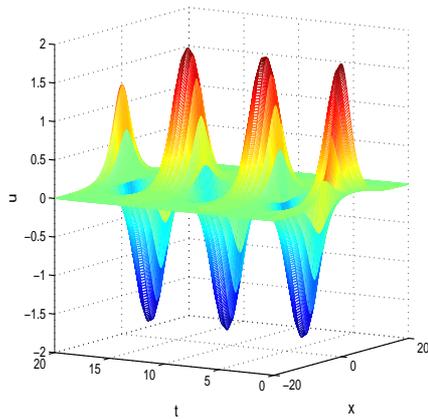


(a) Energy Error: $h = 0.01, N = 400$

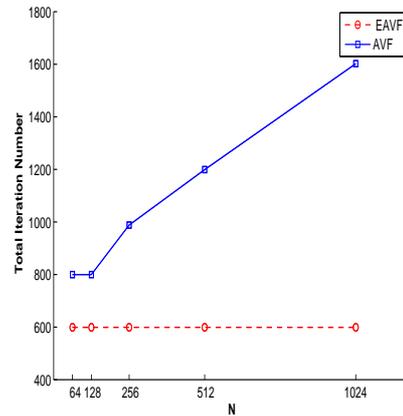


(b) Global Error: $h = 0.01, N = 400$

Fig. 4.1.: The sine-Gordon equation with finite differences semi-discretization: (a) the logarithm of energy error, and (b) the logarithm of global error vs time for AVF and EAVF methods.



(a) Numerical solution: $h = 0.01, N = 400$



(b) Efficiency: $h = 0.01$, maximum iteration number = 1000

Fig. 4.2.: The sine-Gordon equation with finite differences semi-discretization: (a) Numerical solution by EAVF method, and (b) efficiency: the total iteration number against the dimension of spatial discretization.

of the energy errors and the logarithm of the global errors against time t , respectively. The results are shown in Fig. 4.1. The errors of energy and the global errors are comparable for the two schemes. The numerical solution by the EAVF method is shown in Fig. 4.2(a).

In order to illustrate the efficiency of the two schemes, we set the maximum iteration number as 1000 and the error tolerance as 10^{-15} . We apply the two methods to the system in the interval $[0, 2]$ with the stepsize $h = 0.01$. We plot the total iteration number against the dimension of spatial discretization N . The results are shown in Fig. 4.2(b).

Problem 2. We again consider the sine-Gordon equation in Problem 1. Instead of using finite differences for discretization of the spatial derivative in (4.2), we use a spectral discretization with Fourier basis. The derivative u_x can be approximated by discrete Fourier transform (DFT),

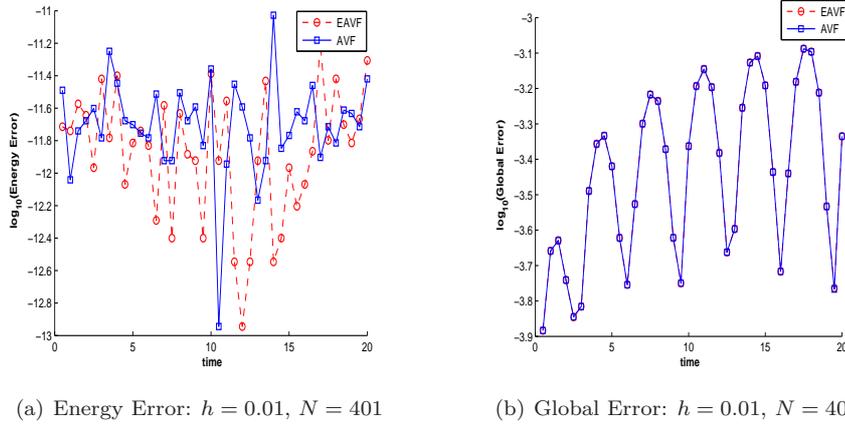


Fig. 4.3.: The sine-Gordon equation with spectral semi-discretization: (a) the logarithm of energy error, and (b) the logarithm of global error vs time for AVF and EAVF methods.

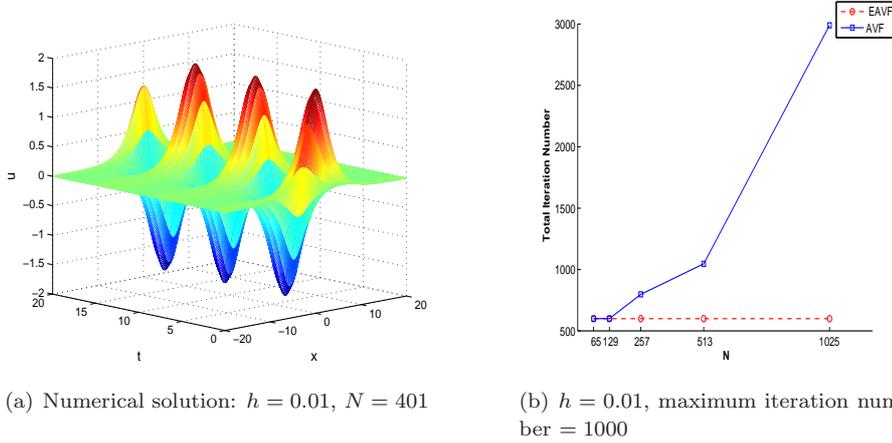


Fig. 4.4.: The sine-Gordon equation with spectral semi-discretization: (a) Numerical solution by EAVF method, and (b) efficiency: the total iteration number against the dimension of spatial discretization.

as $\mathcal{F}_N^{-1}D_N\mathcal{F}_N U$, where \mathcal{F}_N with entries $[\mathcal{F}_N]_{j,k} = e^{-jki2\pi/N}$ is the matrix of DFT coefficients, and we have $[\mathcal{F}_N^{-1}]_{j,k} = \frac{1}{N}e^{jki2\pi/N}$. D_N is a diagonal matrix whose diagonal entries are ([4])

$$\text{diag}(D_N) = \begin{cases} \frac{\pi i}{L} \left[0, 1, 2, \dots, \frac{N-1}{2}, -\frac{N-1}{2}, \dots, -2, -1 \right], & \text{for } N \text{ is odd,} \\ \frac{\pi i}{L} \left[0, 1, 2, \dots, \frac{N}{2} - 1, 0, -\frac{N}{2} + 1, \dots, -2, -1 \right], & \text{for } N \text{ is even.} \end{cases}$$

We follow the notation in Problem 1. (4.2) can be approximated by

$$\bar{G}(U)\Delta x = \left(\sum_{j=0}^{N-1} \frac{1}{2} [\mathcal{F}_N^{-1}D_N\mathcal{F}_N U]_j^2 + (1 - \cos(u_j)) \right) \Delta x.$$

The resulting system of ODEs is given by

$$\frac{d^2U}{dt^2} + MU = f(U), \tag{4.4}$$

where U and $f(U)$ are the same as in Problem 1. M now becomes

$$M = (\mathcal{F}_N^{-1}D_N\mathcal{F}_N)^T (\mathcal{F}_N^{-1}D_N\mathcal{F}_N). \tag{4.5}$$

The system is integrated in the interval $[0, 20]$ with $N = 401$ and $h = 0.01$. First, we set the error tolerance as 10^{-15} for the fixed-point iteration. We plot the logarithm of the energy errors and the logarithm of the global errors against time t , respectively. The results are shown in Fig. 4.3. The numerical solution by the EAVF method is shown in Fig. 4.4(a).

We then set the maximum iteration number as 1000 and the error tolerance as 10^{-15} . We apply the two methods to the system in the interval $[0, 2]$ with the stepsize $h = 0.01$. We plot the total iteration number against the dimension of spatial discretization N . The results are shown in Fig. 4.4(b).

As we can observe from the results, the errors of energy and the global errors are comparable for the two schemes. The total number of iteration of the AVF method grows very fast with the increase of N . However, the total number of iteration of the EAVF method remains almost the same as N grows, which is much less than that of the AVF method. It should be noted that when N is large, the iteration of the AVF method does not converge at some steps within maximum iteration number.

Problem 3. Consider nonlinear 2D wave equation

$$\frac{\partial^2 u}{\partial t^2} = \Delta u - \frac{\partial V(u)}{\partial u}, \quad (x, y) \in [-1, 1] \times [-1, 1], \quad t > 0$$

with $V(u) = u^4/4$. We consider periodic boundary conditions. And the initial conditions are given as

$$u(x, y, 0) = \text{sech}(10x)\text{sech}(10y).$$

The equation is of the type (2.1) with

$$\mathcal{G}[u] = \int_{-1}^1 \int_{-1}^1 \frac{1}{2} \left(\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right) + V(u) dx. \tag{4.6}$$

Following [4], we use spectral elements method to semi-discretize the wave equation. For completeness of the paper, we restate the setup given in [4]. $\mathcal{G}[u]$ is discretized in space with a tensor product Lagrange quadrature formula based on $p + 1$ Gauss-Lobatto-Legendre (GLL) quadrature nodes in each space direction. We obtain

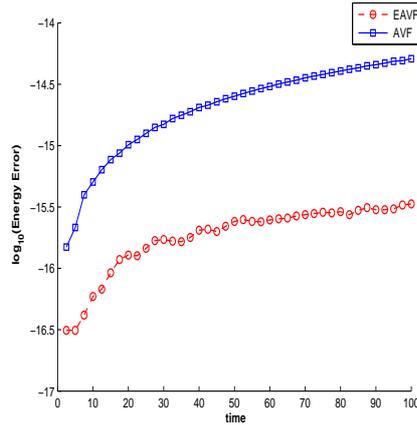
$$\bar{G}(U) = \frac{1}{2} \sum_{j_1=0}^p \sum_{j_2=0}^p w_{j_1} w_{j_2} \left(\left(\sum_{k=0}^p d_{j_1,k} u_{k,j_2} \right)^2 + \left(\sum_{m=0}^p d_{j_2,m} u_{j_1,m} \right)^2 + \frac{1}{2} u_{j_1,j_2}^4 \right),$$

where $d_{j_1,k} = \frac{dl_k(x)}{dx}$, and $l_k(x)$ is the k th Lagrange basis function based on the GLL quadrature nodes x_0, \dots, x_p and with w_0, \dots, w_p the corresponding quadrature weights. The numerical approximation is

$$u_p(x, y, t) = \sum_{k=0}^p \sum_{m=0}^p u_{k,m}(t) l_k(x) l_m(y)$$

with the property $u_p(x_{j_1}, y_{j_2}, t) = u_{j_1, j_2}(t)$. Notice that the quadratic terms with respect to $u_{j_1, j_2}, j_1, j_2 = 0, \dots, p$ in $\bar{G}(U)$ result in the linear terms in the semi-discretized system of ODEs, which will be attributed to MU . Moreover, it can be verified that the matrix M is symmetric and semi-positive.

The system is integrated in the interval $[0, 100]$ with $p = 5$ and $h = 0.05$. The error tolerance of fixed-point iteration is set as 10^{-15} . We show the energy errors in Fig. 4.5. Some snapshots of the numerical solution by EAVF method are shown in Fig. 4.6.



Energy Error: $h = 0.05, p = 5$

Fig. 4.5.: 2D wave equation with spectral elements semi-discretization: the logarithm of energy error vs time for AVF and EAVF methods.

4.3. Dissipative wave equations

In this subsection, we consider the dissipative wave equations given in subsection 4.2.

Problem 4. Consider the dissipative sine-Gordon equation

$$\frac{\partial^2 u}{\partial t^2} + \alpha \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \sin u, \quad t > 0.$$

with $\alpha = 0.1$.

With the same setting as in Problems 1 and 2, we plot the energy curves and the efficiency curves for finite differences and spectral semi-discretization. If the number is very large, we do not plot the points in the figure. The results are shown in Fig. 4.7 and Fig. 4.8. It is shown that the two schemes preserve the decay of energy. And EAVF method is more efficient than AVF method regarding the iteration.

Problem 5. Consider nonlinear 2D dissipative wave equation

$$\frac{\partial^2 u}{\partial t^2} + \alpha \frac{\partial u}{\partial t} = \Delta u - \frac{\partial V(u)}{\partial u}, \quad (x, y) \in [-1, 1] \times [-1, 1], \quad t > 0$$

with $\alpha = 0.1$.

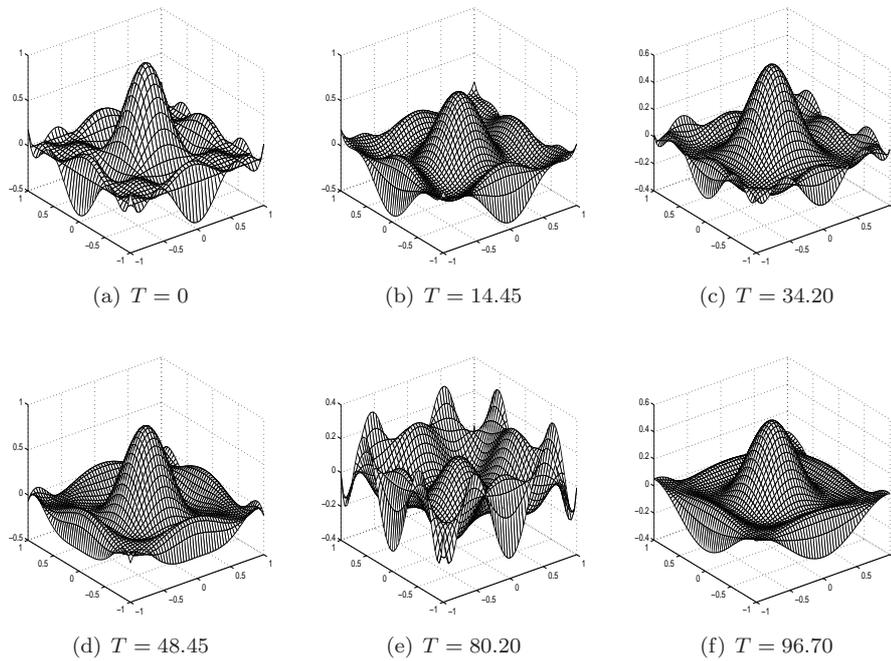
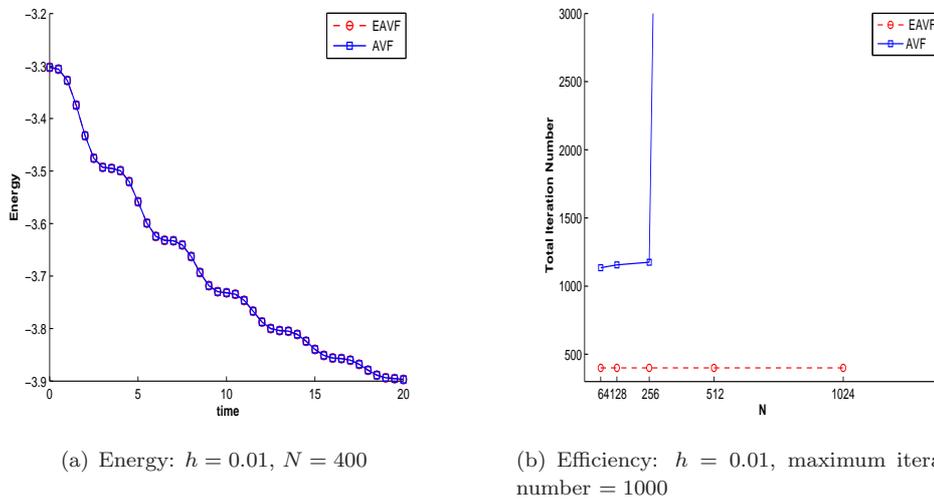


Fig. 4.6.: Snapshots of the solution of the 2D wave equation at different times. EAVF method with the time stepsize $h = 0.05$. Space discretization with six Gauss Lobatto nodes in each spatial direction. Numerical solution interpolated on a equidistant grid of 26 nodes in each spatial direction.

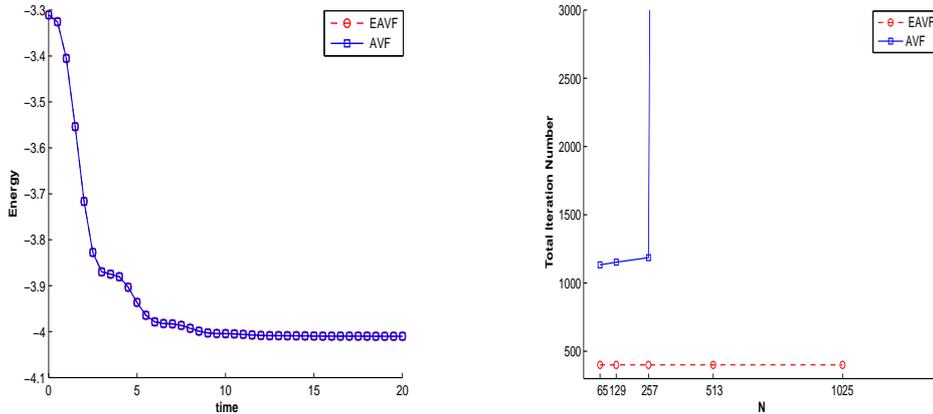


(a) Energy: $h = 0.01$, $N = 400$

(b) Efficiency: $h = 0.01$, maximum iteration number = 1000

Fig. 4.7.: Dissipative sine-Gordon equation with finite differences semi-discretization: (a) Energy vs time, and (b) the total iteration number against the dimension of spatial discretization for AVF and EAVF methods.

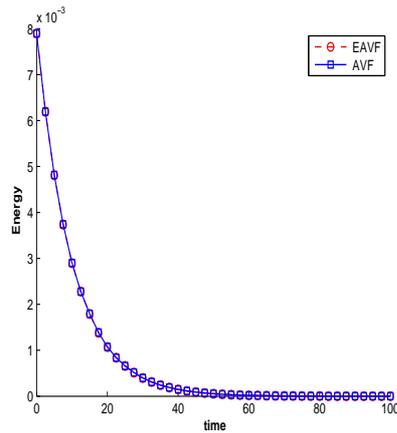
The system is integrated in the interval $[0, 100]$ with $p = 5$ and $h = 0.05$. We plot the energy and some snapshots of the numerical solution by EAVF method in Fig. 4.9 and Fig. 4.10, respectively.



(a) Energy: $h = 0.01$, $N = 401$

(b) Efficiency: $h = 0.01$, maximum iteration number = 1000

Fig. 4.8.: Dissipative sine-Gordon equation with spectral semi-discretization: (a) Energy vs time, and (b) the total iteration number against the dimension of spatial discretization for AVF and EAVF methods.



Energy: $h = 0.05$, $p = 5$

Fig. 4.9.: 2D dissipative wave equation with spectral elements semi-discretization: Energy vs time for AVF and EAVF methods.

Comparing Fig. 4.10 with Fig. 4.6, it is clear that the shapes of the solutions of conservative and dissipative 2D wave equation are similar at the same time step. Due to the damping term, the magnitude of the solution diminishes as time goes which is consistent with the fact that the energy decays in the dissipative case.

5. Conclusions

In this paper, we proposed and analyzed a new approach to designing conservative (dissipative) schemes for nonlinear conservative (dissipative) wave PDEs. Motivated by the idea

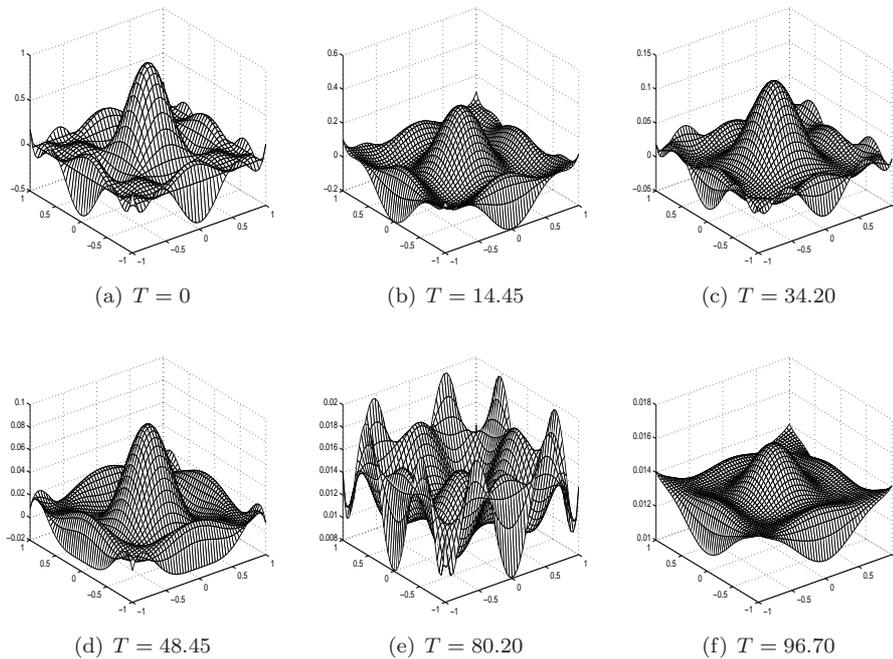


Fig. 4.10.: Snapshots of the solution of the 2D dissipative wave equation at different times. EAVF method with time stepsize $h = 0.05$. Space discretization with six Gauss Lobatto nodes in each space direction. Numerical solution interpolated on a equidistant grid of 26 nodes in each space direction.

in [4], but with some modifications, i.e., we consider directly the original form of wave equations rather than transforming it into a system of first-order PDEs and discretize the functional $\mathcal{G}[u]$ instead of the energy functional $\mathcal{H}[u]$. Using this approach, we obtain a system of second-order ODEs in time. With this framework, the extended AVF method instead of traditional AVF method is applied to the system of second-order ODEs. This procedure presents a linearly-fitted conservative (dissipative) scheme for nonlinear conservative (dissipative) wave equations. The implicit iteration in the new scheme with extended AVF method converges much faster than that of the one with traditional AVF method. In other words, the new scheme is much more efficient in practical applications. The numerical results by comparison between the two schemes illustrate this point clearly.

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