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An extended discrete gradient formula for oscillatory Hamiltonian systems

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Abstract

In this paper, incorporating the idea of the discrete gradient method into the extended Runge–Kutta–Nyström integrator, we derive and analyze an extended discrete gradient formula for the oscillatory Hamiltonian system with the Hamiltonian $H(p, q) = \frac{1}{2}p^T p + \frac{1}{2}q^T Mq + U(q)$, where $q : \mathbb{R} \to \mathbb{R}^d$ represents generalized positions, $p : \mathbb{R} \to \mathbb{R}^d$ represents generalized momenta and $M \in \mathbb{R}^{d\times d}$ is a symmetric and positive semi-definite matrix. The solution of this system is a nonlinear oscillator. Basically, many nonlinear oscillatory mechanical systems with a partitioned Hamiltonian function lend themselves to this approach. The extended discrete gradient formula presented in this paper exactly preserves the energy $H(p, q)$. We derive some properties of the new formula. The convergence is analyzed for the implicit schemes based on the discrete gradient formula, and it turns out that the convergence of the implicit schemes based on the extended discrete gradient formula is independent of $\|M\|$, which is a significant property for the oscillatory Hamiltonian system. Thus, it transpires that a larger step size can be chosen for the new energy-preserving schemes than that for the traditional discrete gradient methods when applied to the oscillatory Hamiltonian system. Illustrative examples show the competence and efficiency of the new schemes in comparison with the traditional discrete gradient methods in the scientific literature.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The design and analysis of numerical integration methods for nonlinear oscillators is an important problem that has received a great deal of attention over the last few years. It is known

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that the traditional approach to achieving numerical integration methods is based on the natural procedure of discretizing the differential equation in such a way as to make the local truncation errors associated with the discretization as small as possible. A relatively new and increasingly important area in numerical integration methods is that of the geometric integrator. 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 or foliations of the system. Geometric 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 [1–3] for recent surveys of this field.

Consider Hamiltonian differential equations

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

where $y = (p^T, q^T)^T$, $q = (q_1, q_2, \dots, q_d)^T$, $p = (p_1, p_2, \dots, p_d)^T$, q_i are the position coordinates and p_i are the momenta for $i = 1, \dots, d$, ∇ is the gradient operator

$$\left(\frac{\partial}{\partial p_1}, \dots, \frac{\partial}{\partial p_d}, \frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_d}\right)^T,$$

and J is the $2d \times 2d$ skew-symmetric matrix

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

It is known that the Hamiltonian $H(y) = H(p, q)$ is the first integral of the system which implies that it is constant along exact solutions of (1). In applications, $H(y)$ is the total energy (sum of kinetic and potential energy), so that this property is equivalent to energy conservation. Thus, for a numerical integration it is interesting to know whether the Hamiltonian remains constant or nearly constant along the numerical solution over very long time intervals.

It has been shown that symplectic numerical integrators approximately conserve the total energy over times that are exponentially long in the step size [4]. Many energy-preserving methods have been developed for (1), such as the discrete gradient methods [5–11] and the Hamiltonian boundary value methods [12–14]. Numerical integration methods based on the discrete gradient formula were proposed many years ago in order to integrate numerically N-body systems of classical mechanics with possible applications in molecular dynamics and celestial mechanics [6]. The discrete gradient method for (1) is written as [8]

$$\frac{y_{n+1} - y_n}{h} = J^{-1}\overline{\nabla} H(y_n, y_{n+1}). \tag{2}$$

For separable Hamiltonian systems with $H(p, q) = T(p) + V(q)$, the method can be expressed as

$$\frac{q_{n+1} - q_n}{h} = \overline{\nabla} T(p_n, p_{n+1}), \qquad \frac{p_{n+1} - p_n}{h} = -\overline{\nabla} V(q_n, q_{n+1}), \tag{3}$$

where $\overline{\nabla} U$ is the discrete gradient of a scalar function U.

In this paper, we are concerned with the energy-preserving integrators for the Hamiltonian system

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

with the Hamiltonian

$$H(p, q) = \tfrac{1}{2} p^T p + \tfrac{1}{2} q^T M q + U(q), \tag{5}$$

where $q : \mathbb{R} \to \mathbb{R}^d$ represents generalized positions, $p : \mathbb{R} \to \mathbb{R}^d$ represents generalized momenta and $M \in \mathbb{R}^{d\times d}$ is a symmetric and positive semi-definite matrix.

It is easy to see that (4) is simply the following oscillatory second-order differential equations:

$$\begin{cases} \ddot{q}(t) + Mq(t) = f(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, & \dot{q}(t_0) = p_0, \end{cases} \tag{6}$$

where $f : \mathbb{R}^d \to \mathbb{R}^d$ is the negative gradient of $U(q)$. These kinds of systems usually arise in various fields of science and technology, such as mechanics, astronomy, quantum physics, molecular biology and engineering.

In recent years, numerical studies of nonlinear effects in physical systems have received much attention and the numerical treatment of oscillatory systems is fundamental for the understanding of nonlinear phenomena. Accordingly, there has been an enormous advancement in dealing with the oscillatory system (6) and some useful approaches to constructing Runge–Kutta–Nyström (RKN)-type integrators have been proposed. We refer to [15–20] for example. Very recently, Wu *et al* [20] took account of the special structure of the system (6) brought by the linear term Mq which leads to the high-frequency oscillation in the solution and formulated a standard form of the multidimensional ERKN (extended RKN) integrators. The ERKN integrators exhibit the correct qualitative behavior much better than the classical RKN methods due to using the special structure of the equation brought by the linear term Mq. For work on this topic, we refer the reader to [19, 21–24].

With this background, taking into account the special structure of the equation brought by the linear term Mq and integrating the idea of the discrete gradient method with the ERKN integrator, we formulate an extended discrete gradient formula for the Hamiltonian system (4).

The outline of this paper is as follows. The preliminaries are given in section 2. In section 3, we derive the extended discrete gradient formula for (4) or (6) which is shown to be energy-preserving. Some other properties of the new formula are also presented in this section. In section 4, the convergence of the fixed-point iteration is analyzed for the implicit integrators. In section 5, the new numerical integration methods are applied to some oscillatory Hamiltonian problems to show the efficiency and robustness of these new energy-preserving integrators in comparison with the traditional discrete gradient methods. The last section focuses on some conclusions and discussions.

2. Preliminaries

This section presents the preliminaries in order to gain an insight into a new class of energy-preserving integrators for the Hamiltonian system (4), equivalently, second-order differential equations (6).

First, we introduce the discrete gradient method. Consider the continuous time systems of a linear-gradient form

$$\dot{y} = L(y)\nabla Q(y), \tag{7}$$

with $L(y)$ being a matrix-valued function which is skew-symmetric for all y. Note that the terminology 'linear-gradient' has nothing to do with whether the system under consideration is linear or not.

The corresponding discrete gradient method for (7) has the following form:

$$\frac{y' - y}{h} = \overline{L}(y, y', h)\overline{\nabla}Q(y, y'), \tag{8}$$

where it is required that $\overline{L}(y, y, 0) = L(y)$ and $\overline{\nabla}Q(y, y) = \nabla Q(y)$ for consistency. Here, $\overline{\nabla}Q$ is a discrete gradient of Q defined as follows (see [25]).

Definition 2.1. *Let Q be a differentiable function. Then $\overline{\nabla} Q$ is a discrete gradient of Q provided it is continuous and satisfies*

$$\begin{cases} \overline{\nabla} Q(y, y') \cdot (y' - y) = Q(y') - Q(y), \\ \overline{\nabla} Q(y, y) = \nabla Q(y). \end{cases} \tag{9}$$

It is obvious that for (1), the discrete gradient method (8) with $y' = y_{n+1}$, $y = y_n$ and $\overline{L} = J^{-1}$ reduces to (2).

In what follows, we give three examples of discrete gradient of $Q(y)$.

- The *mean value discrete gradient* (Harten *et al* [26]):

$$\overline{\nabla}_1 Q(y, y') := \int_0^1 \nabla Q((1-\tau)y + \tau y')\,\mathrm{d}\tau, \quad y \neq y'. \tag{10}$$

- The *midpoint discrete gradient* (Gonzalez [25]):

$$\overline{\nabla}_2 Q(y, y') := \nabla Q\left(\frac{1}{2}(y + y')\right) + \frac{Q(y') - Q(y) - \nabla Q\left(\frac{1}{2}(y+y')\right) \cdot (y' - y)}{|y' - y|^2}(y' - y), \quad y \neq y'. \tag{11}$$

  Both the mean value and the midpoint discrete gradient are second-order approximations to the value of the gradient at the midpoint of the interval $[y, y']$, being exact for linearly varying ∇Q.

- The *coordinate increment discrete gradient* (Itoh and Abe [5]):

$$\overline{\nabla}_3 Q(y, y') := \begin{pmatrix} \dfrac{Q(y_1', y_2, y_3, \ldots, y_d) - Q(y_1, y_2, y_3, \ldots, y_d)}{y_1' - y_1} \\ \dfrac{Q(y_1', y_2', y_3, \ldots, y_d) - Q(y_1', y_2, y_3, \ldots, y_d)}{y_2' - y_2} \\ \vdots \\ \dfrac{Q(y_1', \ldots, y_{d-2}', y_{d-1}', y_d) - Q(y_1', \ldots, y_{d-2}', y_{d-1}, y_d)}{y_{d-1}' - y_{d-1}} \\ \dfrac{Q(y_1', \ldots, y_{d-2}', y_{d-1}', y_d') - Q(y_1', \ldots, y_{d-2}', y_{d-1}', y_d)}{y_d' - y_d} \end{pmatrix}, \tag{12}$$

  in which $0/0$ is understood to be $\partial Q/\partial y_i$.

  The coordinate increment discrete gradient is only a first-order approximation of the gradient at the midpoint of the interval $[y, y']$.

It can be observed that for $T(p) = \frac{1}{2}p^T p$, all three discrete gradients reduce to $\overline{\nabla} T(p, p') = \frac{1}{2}(p + p')$. With the definition, the discrete gradient method for (4) with (5) becomes

$$\frac{q_{n+1} - q_n}{h} = \frac{1}{2}(p_n + p_{n+1}), \qquad \frac{p_{n+1} - p_n}{h} = -\overline{\nabla} V(q_n, q_{n+1}), \tag{13}$$

or equivalently,

$$\begin{aligned} q_{n+1} &= q_n + h p_n - \frac{h^2}{2}\overline{\nabla} V(q_n, q_{n+1}), \\ p_{n+1} &= p_n - h\overline{\nabla} V(q_n, q_{n+1}), \end{aligned} \tag{14}$$

where $\overline{\nabla} V(q_n, q_{n+1})$ is the discrete gradient of $V(q) = \frac{1}{2}q^T M q + U(q)$.

Before going on to describe the extended discrete gradient formula, we define the matrix-valued functions which appeared first in [19]

$$\phi_l(M) := \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+l)!}, \quad l = 0, 1, \dots. \tag{15}$$

Let

$$W = \begin{pmatrix} 0 & I \\ -M & 0 \end{pmatrix}, \quad y = \begin{pmatrix} q \\ p \end{pmatrix}, \quad G(y) = \begin{pmatrix} 0 \\ -\nabla U(q) \end{pmatrix}, \quad y_0 = \begin{pmatrix} q_0 \\ p_0 \end{pmatrix},$$

then the Hamiltonian system (4) can be rewritten as

$$\begin{cases} \dot{y} = Wy + G(y), \\ y(t_0) = y_0. \end{cases} \tag{16}$$

From the well-known variation-of-constant formula, the solution of the system (16) has the form

$$y(t) = \exp((t-t_0)W)y_0 + \int_{t_0}^{t} \exp((t-\xi)W)G(y(\xi))\,\mathrm{d}\xi. \tag{17}$$

Here and hereafter, the integral of a matrix-valued or vector-valued function is understood componentwise.

By the definition of the ϕ-functions, we have the following formula (see [19]):

$$\exp((t-t_0)W) = \begin{pmatrix} \phi_0((t-t_0)^2M) & (t-t_0)\phi_1((t-t_0)^2M) \\ -(t-t_0)M\phi_1((t-t_0)^2M) & \phi_0((t-t_0)^2M) \end{pmatrix}. \tag{18}$$

Substituting (18) into (17) gives

$$\begin{aligned} \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} &= \begin{pmatrix} \phi_0((t-t_0)^2M) & (t-t_0)\phi_1((t-t_0)^2M) \\ -(t-t_0)M\phi_1((t-t_0)^2M) & \phi_0((t-t_0)^2M) \end{pmatrix} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \\ &\quad + \int_{t_0}^{t} \begin{pmatrix} \phi_0((t-\xi)^2M) & (t-\xi)\phi_1((t-\xi)^2M) \\ -(t-\xi)M\phi_1((t-\xi)^2M) & \phi_0((t-\xi)^2M) \end{pmatrix} \begin{pmatrix} 0 \\ -\nabla U(q(\xi)) \end{pmatrix} \mathrm{d}\xi \\ &= \begin{pmatrix} \phi_0((t-t_0)^2M)q_0 + (t-t_0)\phi_1((t-t_0)^2M)p_0 \\ \phi_0((t-t_0)^2M)p_0 - (t-t_0)M\phi_1((t-t_0)^2M)q_0 \end{pmatrix} \\ &\quad - \begin{pmatrix} \displaystyle\int_{t_0}^{t} (t-\xi)\phi_1((t-\xi)^2M)\nabla U(q(\xi))\,\mathrm{d}\xi \\ \displaystyle\int_{t_0}^{t} \phi_0((t-\xi)^2M)\nabla U(q(\xi))\,\mathrm{d}\xi \end{pmatrix}, \end{aligned}$$

which further gives

$$\begin{aligned} q(t) &= \phi_0((t-t_0)^2M)q_0 + (t-t_0)\phi_1((t-t_0)^2M)p_0 \\ &\qquad - \int_{t_0}^{t} (t-\xi)\phi_1((t-\xi)^2M)\nabla U(q(\xi))\,\mathrm{d}\xi, \\ p(t) &= -(t-t_0)M\phi_1((t-t_0)^2M)q_0 + \phi_0((t-t_0)^2M)p_0 \\ &\qquad - \int_{t_0}^{t} \phi_0((t-\xi)^2M)\nabla U(q(\xi))\,\mathrm{d}\xi. \end{aligned} \tag{19}$$

It follows immediately from (19) that

$$\begin{aligned} q(t_n+h) &= \phi_0(K)q(t_n) + h\phi_1(K)p(t_n) - h^2\int_0^1 (1-z)\phi_1((1-z)^2K)\nabla U(q(t_n+hz))\,\mathrm{d}z, \\ p(t_n+h) &= -hM\phi_1(K)q(t_n) + \phi_0(K)p(t_n) - h\int_0^1 \phi_0((1-z)^2K)\nabla U(q(t_n+hz))\,\mathrm{d}z, \end{aligned} \tag{20}$$

where $K = h^2M$. In the particular case where $\nabla U(q) \equiv \nabla U_0$ is constant, (20) becomes

$$\begin{aligned} q(t_n + h) &= \phi_0(K)q(t_n) + h\phi_1(K)p(t_n) - h^2\phi_2(K)\nabla U_0, \\ p(t_n + h) &= -hM\phi_1(K)q(t_n) + \phi_0(K)p(t_n) - h\phi_1(K)\nabla U_0, \end{aligned} \tag{21}$$

which gives the exact solution of the Hamiltonian system (4).

3. An extended discrete gradient formula based on ERKN integrators and its properties

In this section, we give and analyze an extended discrete gradient formula based on ERKN integrators for the Hamiltonian system (4).

From formulas (20) and (21), we consider the following extended discrete gradient formula:

$$\begin{aligned} q_{n+1} &= \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\overline{\nabla}U(q_n, q_{n+1}), \\ p_{n+1} &= -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K)\overline{\nabla}U(q_n, q_{n+1}), \end{aligned} \tag{22}$$

where h is the step size, $K = h^2M$, $\overline{\nabla}U(q_n, q_{n+1})$ is the discrete gradient of $U(q)$. Each of the three discrete gradients $\overline{\nabla}_1U(q_n, q_{n+1})$, $\overline{\nabla}_2U(q_n, q_{n+1})$ and $\overline{\nabla}_3U(q_n, q_{n+1})$ introduced in section 2 can be chosen as $\overline{\nabla}U(q_n, q_{n+1})$.

For the extended discrete gradient formula (22), we present the following important theorem.

Theorem 3.1. *Formula (22) exactly preserves the Hamiltonian H defined by (5).*

Proof. We compute

$$H(p_{n+1}, q_{n+1}) = \tfrac{1}{2}p_{n+1}^T p_{n+1} + \tfrac{1}{2}q_{n+1}^T M q_{n+1} + U(q_{n+1}). \tag{23}$$

Using the symmetry of M and commutativity of M and all the $\phi_l(K)$ and inserting (22) into (23), with a tedious computation we obtain

$$\begin{aligned} H(p_{n+1}, q_{n+1}) = {} & \tfrac{1}{2}p_n^T\big(\phi_0^2(K) + K\phi_1^2(K)\big)p_n + \tfrac{1}{2}q_n^T M\big(\phi_0^2(K) + K\phi_1^2(K)\big)q_n \\ & + q_n^T K\big(\phi_1(K)^2 - \phi_0(K)\phi_2(K)\big)\overline{\nabla}U(q_n, q_{n+1}) \\ & - hp_n^T\big(\phi_0(K)\phi_1(K) + K\phi_1(K)\phi_2(K)\big)\overline{\nabla}U(q_n, q_{n+1}) \\ & + \tfrac{1}{2}h^2\overline{\nabla}U(q_n, q_{n+1})^T\big(\phi_1(K)^2 + K\phi_2(K)^2\big)\overline{\nabla}U(q_n, q_{n+1}) + U(q_{n+1}). \end{aligned} \tag{24}$$

From the definition of $\phi_i(K)$, it can be shown that

$$\begin{aligned} &\phi_0^2(K) + K\phi_1^2(K) = I, \qquad K\big(\phi_1(K)^2 - \phi_0(K)\phi_2(K)\big) = I - \phi_0(K), \\ &\phi_1(K)^2 + K\phi_2(K)^2 = 2\phi_2(K), \qquad \phi_0(K) + K\phi_2(K) = I, \end{aligned} \tag{25}$$

where I is the $d \times d$ identity matrix.

Substituting (25) into (24) gives

$$\begin{aligned} H(p_{n+1}, q_{n+1}) = {} & \tfrac{1}{2}p_n^T p_n + \tfrac{1}{2}q_n^T M q_n + q_n^T\big(I - \phi_0(K)\big)\overline{\nabla}U(q_n, q_{n+1}) \\ & - hp_n^T\phi_1(K)\overline{\nabla}U(q_n, q_{n+1}) \\ & + h^2\overline{\nabla}U(q_n, q_{n+1})^T\phi_2(K)\overline{\nabla}U(q_n, q_{n+1}) + U(q_{n+1}). \end{aligned} \tag{26}$$

With the definition of the discrete gradient and the first equation of (22), (26) becomes

$$\begin{aligned} H(p_{n+1}, q_{n+1}) &= \tfrac{1}{2}p_n^T p_n + \tfrac{1}{2}q_n^T M q_n + (q_n - (\phi_0(K)q_n + h\phi_1(K)p_n \\ &\quad - h^2\phi_2(K)\overline{\nabla}U(q_n, q_{n+1})))^T\overline{\nabla}U(q_n, q_{n+1}) + U(q_{n+1}) \\ &= \tfrac{1}{2}p_n^T p_n + \tfrac{1}{2}q_n^T M q_n + \big(q_n - q_{n+1}\big)^T\overline{\nabla}U(q_n, q_{n+1}) + U(q_{n+1}) \\ &= \tfrac{1}{2}p_n^T p_n + \tfrac{1}{2}q_n^T M q_n + U(q_n) \\ &= H(p_n, q_n). \end{aligned} \tag{27}$$

The proof is complete. □

Remark 1. It is noted that in the particular case of $M = \mathbf{0}$, the $d \times d$ zero matrix, namely $H(p, q) = \frac{1}{2}p^T p + U(q)$, formula (22) reduces to the traditional discrete gradient method (13). In fact, the choice of $M = \mathbf{0}$ in (22) gives

$$q_{n+1} = q_n + hp_n - \tfrac{1}{2}h^2\overline{\nabla}U(q_n, q_{n+1}), \qquad p_{n+1} = p_n - h\overline{\nabla}U(q_n, q_{n+1}), \tag{28}$$

or equivalently,

$$q_{n+1} = q_n + \tfrac{1}{2}h(p_n + p_{n+1}), \qquad p_{n+1} = p_n - h\overline{\nabla}U(q_n, q_{n+1}), \tag{29}$$

which is exactly the same as (13).

In what follows, we go further on studying the extended discrete gradient formula (22) and give some other properties related to the formula.

First, we consider the classical algebraic order of (22). An integration formula has order r, if for any smooth problem under consideration, the local truncation errors of the formula satisfy

$$e_{n+1} := q(t_{n+1}) - q_{n+1} = \mathcal{O}(h^{r+1}) \qquad \text{and} \qquad e'_{n+1} := p(t_{n+1}) - p_{n+1} = \mathcal{O}(h^{r+1}),$$

where $q(t_{n+1})$ and $p(t_{n+1})$ denote the values of the exact solution of the problem and its first derivative at $t_{n+1} = t_n + h$, respectively, and q_{n+1} and p_{n+1} express the one-step numerical results obtained by the formula under the local assumptions $q_n = q(t_n)$ and $p_n = p(t_n)$.

Theorem. *Assume that $\overline{\nabla}U(q, q')$ is at least a first-order approximation to the gradient of $U(q)$ at the midpoint of the interval $[q, q']$; then the extended discrete gradient formula (22) is of order 2.*

Proof. By (20) and (22), we have

$$q(t_{n+1}) - q_{n+1} = h^2\int_0^1 -(1-z)\phi_1((1-z)^2K)\nabla U(q(t_n + hz)) + h^2\phi_2(K)\overline{\nabla}U(q_n, q_{n+1})\,\mathrm{d}z. \tag{30}$$

The first equation of (22) gives

$$q_{n+1} - q_n = (\phi_0(K) - I)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\overline{\nabla}U(q_n, q_{n+1}).$$

From $\phi_0(K) - I = \mathcal{O}(h^2)$, it follows that

$$q_{n+1} - q_n = \mathcal{O}(h). \tag{31}$$

Under the local assumption $q_n = q(t_n)$, we have

$$q(t_n + hz) - q_n = \mathcal{O}(h), \qquad 0 \leqslant z \leqslant 1. \tag{32}$$

From (31) and (32), we obtain

$$q(t_n + hz) - \frac{q_n + q_{n+1}}{2} = \mathcal{O}(h), \qquad 0 \leqslant z \leqslant 1. \tag{33}$$

Thus, with (33) and the assumption of the theorem, (30) becomes

$$\begin{aligned} q(t_{n+1}) - q_{n+1} &= h^2 \int_0^1 -(1-z)\phi_1((1-z)^2K)\left(\nabla U\left(\frac{q_n+q_{n+1}}{2}\right)+\mathcal{O}(h)\right) \\ &\quad + \phi_2(K)\left(\nabla U\left(\frac{q_n+q_{n+1}}{2}\right)+\mathcal{O}(h)\right)\mathrm{d}z \\ &= h^2\int_0^1 (-(1-z)\phi_1((1-z)^2K)+\phi_2(K))\nabla U\left(\frac{q_n+q_{n+1}}{2}\right)+\mathcal{O}(h)\,\mathrm{d}z \\ &= \mathcal{O}(h^3). \end{aligned}$$

Similarly, we obtain $p(t_{n+1}) - p_{n+1} = \mathcal{O}(h^3)$. □

It is known that the symmetry of a method is very important in long-term integration. The definition of symmetry of a method is given below (see [1]).

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

With the definition of symmetry, a method is symmetric if exchanging $n+1 \leftrightarrow n,\ h \leftrightarrow -h$ leaves the method unaltered. Symmetric methods have even-order algebraic accuracy (see [1]).

In what follows, we show that the extended discrete gradient formula (22) is symmetric.

Theorem 3.3. *The extended discrete gradient formula (22) is symmetric provided $\overline{\nabla}U$ in (22) satisfies the assumption $\overline{\nabla}U(q,q') = \overline{\nabla}U(q',q)$ for all q and q'.*

Proof. Exchanging $q_{n+1} \leftrightarrow q_n,\ p_{n+1} \leftrightarrow p_n$ and replacing h by $-h$ in (22) give

$$\begin{aligned} q_n &= \phi_0(K)q_{n+1} - h\phi_1(K)p_{n+1} - h^2\phi_2(K)\overline{\nabla}U(q_{n+1},q_n), \\ p_n &= hM\phi_1(K)q_{n+1} + \phi_0(K)p_{n+1} + h\phi_1(K)\overline{\nabla}U(q_{n+1},q_n). \end{aligned} \tag{34}$$

Multiplying both sides of the two equations in (34) by ϕ_0 and ϕ_1, respectively, and with some computation, we obtain

$$\begin{aligned} q_{n+1} &= \phi_0(K)q_n + h\phi_1(K)p_n - h^2\big(\phi_1^2(K)-\phi_0(K)\phi_2(K)\big)\overline{\nabla}U(q_{n+1},q_n), \\ p_{n+1} &= -hM\phi_1(K)q_n + \phi_0(K)p_n - h(K\phi_1(K)\phi_2(K)+\phi_0(K)\phi_1(K))\overline{\nabla}U(q_{n+1},q_n). \end{aligned} \tag{35}$$

Since $\phi_1^2(K) - \phi_0(K)\phi_2(K) = \phi_2(K)$ and $K\phi_1(K)\phi_2(K) + \phi_0(K)\phi_1(K) = \phi_1(K)$, we obtain

$$\begin{aligned} q_{n+1} &= \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\overline{\nabla}U(q_{n+1},q_n), \\ p_{n+1} &= -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K)\overline{\nabla}U(q_{n+1},q_n), \end{aligned} \tag{36}$$

which shows that formula (22) is symmetric under the assumption. □

Remark 2. It should be noted that all the three discrete gradients $\overline{\nabla}_1U, \overline{\nabla}_2U, \overline{\nabla}_3U$ satisfy the assumption of theorem 3.3.

4. Convergence of the fixed-point iteration for the implicit scheme in the discrete gradient formula

The previous section derives the extended discrete gradient formula (22) and presents some properties. In this section, using the discrete gradients given in section 2, we propose three practical schemes based on the extended discrete gradient formula (22) for the Hamiltonian system (4).

- MVDS (mean value discrete gradient):

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\displaystyle\int_0^1 \nabla U((1-\tau)q_n + \tau q_{n+1})\,\mathrm{d}\tau, \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K)\displaystyle\int_0^1 \nabla U((1-\tau)q_n + \tau q_{n+1})\,\mathrm{d}\tau. \end{cases} \tag{37}$$

- MDS (midpoint discrete gradient):

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\Bigg(\nabla U\left(\dfrac{1}{2}(q_n + q_{n+1})\right) \\ \qquad + \dfrac{U(q_{n+1}) - U(q_n) - \nabla U\left(\frac{1}{2}(q_n+q_{n+1})\right)\cdot(q_{n+1}-q_n)}{|q_{n+1}-q_n|^2}(q_{n+1}-q_n)\Bigg), \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K)\Bigg(\nabla U\left(\dfrac{1}{2}(q_n + q_{n+1})\right) \\ \qquad + \dfrac{U(q_{n+1}) - U(q_n) - \nabla U\left(\frac{1}{2}(q_n+q_{n+1})\right)\cdot(q_{n+1}-q_n)}{|q_{n+1}-q_n|^2}(q_{n+1}-q_n)\Bigg). \end{cases} \tag{38}$$

- CIDS (coordinate increment discrete gradient):

$$\begin{cases} q_{n+1} = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\overline{\nabla}U(q_n, q_{n+1}), \\ p_{n+1} = -hM\phi_1(K)q_n + \phi_0(K)p_n - h\phi_1(K)\overline{\nabla}U(q_n, q_{n+1}), \end{cases} \tag{39}$$

with

$$\overline{\nabla}U(q_n, q_{n+1}) := \begin{pmatrix} \dfrac{U\left(q_{n+1}^1, q_n^2, q_n^3, \ldots, q_n^d\right) - U\left(q_n^1, q_n^2, q_n^3, \ldots, q_n^d\right)}{q_{n+1}^1 - q_n^1} \\ \dfrac{U\left(q_{n+1}^1, q_{n+1}^2, q_n^3, \ldots, q_n^d\right) - U\left(q_{n+1}^1, q_n^2, q_n^3, \ldots, q_n^d\right)}{q_{n+1}^2 - q_n^2} \\ \vdots \\ \dfrac{U\left(q_{n+1}^1, \ldots, q_{n+1}^{d-2}, q_{n+1}^{d-1}, q_n^d\right) - U\left(q_{n+1}^1, \ldots, q_{n+1}^{d-2}, q_n^{d-1}, q_n^d\right)}{q_{n+1}^{d-1} - q_n^{d-1}} \\ \dfrac{U\left(q_{n+1}^1, \ldots, q_{n+1}^{d-2}, q_{n+1}^{d-1}, q_{n+1}^d\right) - U\left(q_{n+1}^1, \ldots, q_{n+1}^{d-2}, q_{n+1}^{d-1}, q_n^d\right)}{q_{n+1}^d - q_n^d} \end{pmatrix}, \tag{40}$$

where q^i is the ith component of q.

The corresponding original methods of the above three methods are given by

$$\begin{cases} q_{n+1} = q_n + hp_n - \dfrac{h^2}{2}\displaystyle\int_0^1 \nabla V((1-\tau)q_n + \tau q_{n+1})\,\mathrm{d}\tau, \\ p_{n+1} = p_n - h\displaystyle\int_0^1 \nabla V((1-\tau)q_n + \tau q_{n+1})\,\mathrm{d}\tau, \end{cases} \tag{41}$$

$$\begin{cases} q_{n+1} = q_n + hp_n - \dfrac{h^2}{2}\Bigg(\nabla V\left(\dfrac{1}{2}(q_n + q_{n+1})\right) \\ \quad + \dfrac{V(q_{n+1}) - V(q_n) - \nabla V\left(\frac{1}{2}(q_n + q_{n+1})\right)\cdot(q_{n+1} - q_n)}{|q_{n+1} - q_n|^2}(q_{n+1} - q_n)\Bigg), \\ p_{n+1} = p_n - h\Bigg(\nabla V\left(\dfrac{1}{2}(q_n + q_{n+1})\right) \\ \quad + \dfrac{V(q_{n+1}) - V(q_n) - \nabla V\left(\frac{1}{2}(q_n + q_{n+1})\right)\cdot(q_{n+1} - q_n)}{|q_{n+1} - q_n|^2}(q_{n+1} - q_n)\Bigg) \end{cases} \tag{42}$$

and

$$\begin{cases} q_{n+1} = q_n + hp_n - \dfrac{h^2}{2}\overline{\nabla} V(q_n, q_{n+1}), \\ p_{n+1} = p_n - h\overline{\nabla} V(q_n, q_{n+1}) \end{cases} \tag{43}$$

respectively, where $V(q) = \frac{1}{2}q^T Mq + U(q)$ and $\overline{\nabla} V(q_n, q_{n+1})$ is the same as (40).

Substituting $V(q) = \frac{1}{2}q^T Mq + U(q)$ into (41), (42) and (43), respectively, yields the following three schemes.

- MVDS0:

$$\begin{cases} q_{n+1} = q_n + hp_n - \dfrac{h^2}{2}\left(\dfrac{1}{2}M(q_n + q_{n+1}) + \displaystyle\int_0^1 \nabla U((1-\tau)q_n + \tau q_{n+1})\,\mathrm{d}\tau\right), \\ p_{n+1} = p_n - h\left(\dfrac{1}{2}M(q_n + q_{n+1}) + \displaystyle\int_0^1 \nabla U((1-\tau)q_n + \tau q_{n+1})\,\mathrm{d}\tau\right). \end{cases} \tag{44}$$

- MDS0:

$$\begin{cases} q_{n+1} = q_n + hp_n - \dfrac{h^2}{2}\Bigg(\dfrac{1}{2}M(q_n + q_{n+1}) + \nabla U\left(\dfrac{1}{2}(q_n + q_{n+1})\right) \\ \quad + \dfrac{U(q_{n+1}) - U(q_n) - \nabla U\left(\frac{1}{2}(q_n + q_{n+1})\right)\cdot(q_{n+1} - q_n)}{|q_{n+1} - q_n|^2}(q_{n+1} - q_n)\Bigg), \\ p_{n+1} = p_n - h\Bigg(\dfrac{1}{2}M(q_n + q_{n+1}) + \nabla U\left(\dfrac{1}{2}(q_n + q_{n+1})\right) \\ \quad + \dfrac{U(q_{n+1}) - U(q_n) - \nabla U\left(\frac{1}{2}(q_n + q_{n+1})\right)\cdot(q_{n+1} - q_n)}{|q_{n+1} - q_n|^2}(q_{n+1} - q_n)\Bigg). \end{cases} \tag{45}$$

- CIDS0:

$$\begin{cases} q_{n+1} = q_n + hp_n - \dfrac{h^2}{2}\left(\dfrac{1}{2}M(q_n + q_{n+1}) + \overline{\nabla} U(q_n, q_{n+1})\right), \\ p_{n+1} = p_n - h\left(\dfrac{1}{2}M(q_n + q_{n+1}) + \overline{\nabla} U(q_n, q_{n+1})\right), \end{cases} \tag{46}$$

  where $\overline{\nabla} U(q_n, q_{n+1})$ is defined by (40).

The integrals in (37) and (44) can be approximated by quadrature formulas, in such a way we can obtain the corresponding numerical integration schemes. We note that these schemes are all implicit and require iterative computation, in general. In this paper, we use the well-known fixed-point iteration for these implicit schemes.

In what follows, we analyze the convergence of the fixed-point iteration for the formulas. First, we consider the one-dimensional case.

In the one-dimensional case, the Hamiltonian system (4) reduces to

$$\begin{cases} \dot{q} = p, \quad \dot{p} = -\omega^2 q - \dfrac{\mathrm{d}U}{\mathrm{d}q}, \quad \omega > 0, \quad t \in [t_0, T], \\ q(t_0) = q_0, \quad p(t_0) = p_0, \end{cases} \tag{47}$$

and the Hamiltonian reduces to

$$H(p,q) = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2 q^2 + U(q).$$

The ϕ-functions $\phi_0(K), \phi_1(K)$ and $\phi_2(K)$ in the formulas reduce to $\cos(\nu)$, $\mathrm{sinc}(\nu)$ and $\frac{1}{2}\mathrm{sinc}^2(\frac{\nu}{2})$, respectively, where $\nu = h\omega$, $\mathrm{sinc}(\xi) = \frac{\sin(\xi)}{\xi}$. In this case, all the three new energy-preserving schemes and the three corresponding original ones given in this section for (4) reduce to the following two schemes:

$$\begin{cases} q_{n+1} = \cos(\nu) q_n + h\,\mathrm{sinc}(\nu) p_n - \dfrac{h^2}{2}\mathrm{sinc}^2\left(\dfrac{\nu}{2}\right)\dfrac{U(q_{n+1}) - U(q_n)}{q_{n+1} - q_n}, \\ p_{n+1} = -h\sin(\nu) q_n + \cos(\nu) p_n - h\,\mathrm{sinc}(\nu)\dfrac{U(q_{n+1}) - U(q_n)}{q_{n+1} - q_n}, \end{cases} \tag{48}$$

$$\begin{cases} q_{n+1} = q_n + h p_n - \dfrac{h^2}{2}\left(\dfrac{1}{2}\omega^2 (q_{n+1} + q_n) + \dfrac{U(q_{n+1}) - U(q_n)}{q_{n+1} - q_n}\right), \\ p_{n+1} = p_n - h\left(\dfrac{1}{2}\omega^2 (q_{n+1} + q_n) + \dfrac{U(q_{n+1}) - U(q_n)}{q_{n+1} - q_n}\right). \end{cases} \tag{49}$$

We assume that $U(q)$ is twice continuously differentiable. For fixed h, q_n and p_n, the first equation of (48) is a nonlinear equation with respect to q_{n+1}. Let

$$F(q) = \cos(\nu) q_n + h\,\mathrm{sinc}(\nu) p_n - \frac{h^2}{2}\mathrm{sinc}^2\left(\frac{\nu}{2}\right)\frac{U(q) - U(q_n)}{q - q_n}.$$

Then q_{n+1} is a fixed point of $F(q)$ and we have

$$\begin{aligned} |F(q) - F(q')| &= \left|\frac{h^2}{2}\mathrm{sinc}^2\left(\frac{\nu}{2}\right)\right| \left|\frac{U(q) - U(q_n)}{q - q_n} - \frac{U(q') - U(q_n)}{q' - q_n}\right| \\ &= \left|\frac{h^2}{2}\mathrm{sinc}^2\left(\frac{\nu}{2}\right)\right| \left|\int_0^1 U'((1-\tau)q_n + \tau q) - U'((1-\tau)q_n + \tau q')\,\mathrm{d}\tau\right| \\ &= \left|\frac{h^2}{2}\mathrm{sinc}^2\left(\frac{\nu}{2}\right)\right| \left|\int_0^1 \int_0^1 U''((1-\tau)q_n + (1-s)\tau q' + s\tau q') \right. \\ &\quad \left. \times\ \tau(q - q')\,\mathrm{d}s\,\mathrm{d}\tau\right| \\ &\leqslant \frac{h^2}{4}\max_{\xi} |U''(\xi)||q - q'|. \end{aligned} \tag{50}$$

By the fixed-point theorem, if $\frac{h^2}{4}\max\limits_{\xi} |U''(\xi)| < c < 1$, then the fixed-point iteration for the first equation with respect to q_{n+1} in (48) is convergent. The important point here is that the convergence of the fixed-point iteration for (48) is independent of the frequency ω. Similarly, for the first equation of (49), let

$$G(q) = q_n + h p_n - \frac{h^2}{2}\left(\frac{1}{2}\omega^2 (q + q_n) + \frac{U(q) - U(q_n)}{q - q_n}\right);$$

then

$$
\begin{aligned}
|G(q)-G(q')| &= \frac{h^2}{2}\left|\frac{1}{2}\omega^2(q-q') + \frac{U(q)-U(q_n)}{q-q_n} - \frac{U(q')-U(q_n)}{q'-q_n}\right| \\
&= \frac{h^2}{2}\left|\frac{1}{2}\omega^2(q-q') + \int_0^1 U'((1-\tau)q_n+\tau q) - U'((1-\tau)q_n+\tau q')\,\mathrm{d}\tau\right| \\
&= \frac{h^2}{2}\left|\frac{1}{2}\omega^2(q-q') + \int_0^1\int_0^1 U''((1-\tau)q_n + (1-s)\tau q' + s\tau q') \right.\\
&\quad \left. \times\ \tau(q-q')\,\mathrm{d}s\,\mathrm{d}\tau\right| \\
&= \frac{h^2}{2}\left|\frac{1}{2}\omega^2 + \int_0^1\int_0^1 U''\big((1-\tau)q_n + (1-s)\tau q' + s\tau q'\big)\tau\,\mathrm{d}s\mathrm{d}\tau\right| |q-q'|. \\
&\leqslant \frac{h^2}{4}\left(\omega^2 + \max_{\xi}|U''(\xi)|\right)|q-q'|.
\end{aligned} \tag{51}
$$

Thus, if $\frac{h^2}{4}\big(\omega^2 + \max_{\xi}|U''(\xi)|\big) < c < 1$, then the fixed-point iteration for the first equation with respect to q_{n+1} in the scheme (49) is convergent. We note that the convergence of the fixed-point iteration for (49) is dependent on the frequency ω.

For the multidimensional case, we only consider methods (37) and (44). The analysis for the others can be made in a similar way.

In what follows, we use the Euclidean norm and its induced matrix norm (spectral norm) and denote them by $\|\cdot\|$. Similar to the one-dimensional case, in (37), let the right-hand side of the first equation be $R(q_{n+1})$, where

$$
R(q) = \phi_0(K)q_n + h\phi_1(K)p_n - h^2\phi_2(K)\int_0^1 \nabla U((1-\tau)q_n+\tau q)\,\mathrm{d}\tau,
$$

and let the right-hand side of the first equation in (44) be $I(q_{n+1})$, where

$$
I(q) = q_n + hp_n - \frac{h^2}{2}\left(\frac{1}{2}M(q_n+q) + \int_0^1 \nabla U((1-\tau)q_n+\tau q)\,\mathrm{d}\tau\right).
$$

Then

$$
\begin{aligned}
\|R(q)-R(q')\| &= h^2\left\|\phi_2(K)\int_0^1 U'((1-\tau)q_n+\tau q) - U'((1-\tau)q_n+\tau q')\,\mathrm{d}\tau\right\| \\
&= h^2\left\|\phi_2(K)\int_0^1\int_0^1 U''((1-\tau)q_n+(1-s)\tau q'+s\tau q)\tau(q-q')\,\mathrm{d}s\,\mathrm{d}\tau\right\| \\
&\leqslant \frac{h^2}{2}\|\phi_2(K)\|\max_{\xi}\|\nabla^2 U(\xi)\|\|q-q'\| \\
&\leqslant \frac{h^2}{4}\max_{\xi}\|\nabla^2 U(\xi)\|\|q-q'\|;
\end{aligned} \tag{52}
$$

the last inequality is due to the symmetry of M and the definition of $\phi_2(K)$:

$$
\begin{aligned}
\|I(q)-I(q')\| &= \frac{h^2}{2}\left\|\frac{1}{2}M(q-q') + \int_0^1 U'((1-\tau)q_n+\tau q) - U'((1-\tau)q_n+\tau q')\,\mathrm{d}\tau\right\| \\
&= \frac{h^2}{2}\left\|\frac{1}{2}M(q-q') + \int_0^1\int_0^1 U''((1-\tau)q_n+(1-s)\tau q'+s\tau q)\right. \\
&\quad \left. \times\ \tau(q-q')\,\mathrm{d}s\,\mathrm{d}\tau\right\|
\end{aligned}
$$

$$= \frac{h^2}{2}\left\| \frac{1}{2}M + \int_0^1 \int_0^1 U''((1-\tau)q_n + (1-s)\tau q' + s\tau q)\tau \, \mathrm{d}s \, \mathrm{d}\tau \right\| \|q - q'\|$$

$$\leqslant \frac{h^2}{4}\left(\|M\| + \max_{\xi} \|\nabla^2 U(\xi)\|\right)\|q - q'\|. \tag{53}$$

Comparing (52) with (53), it can be observed that the fixed-point iteration of the extended discrete gradient schemes has a larger convergence domain than that of the traditional discrete gradient schemes, especially, for the case $\|\nabla^2 U\| \ll \|M\|$, where $\nabla^2 U$ is the Hessian matrix of U. Also, it is clear from (53) that the convergence of the fixed-point iteration of the traditional discrete gradient methods depends on $\|M\|$, and the larger the $\|M\|$, the smaller the required step size, whereas it is significant to note from (52) that the convergence of the fixed-point iteration for the implicit schemes based on the extended discrete gradient formula (22) is independent of $\|M\|$.

5. Numerical experiments

In what follows, we apply the methods derived in this paper to the following three problems and show the efficiency. All the computations and graphics are performed in MATLAB 7 in IEEE double precision arithmetic.

Problem 1. Consider the Duffing equation

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

with $0 \leqslant k < \omega$. The problem is a Hamiltonian system with

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

The analytic solution of this initial value problem is given by

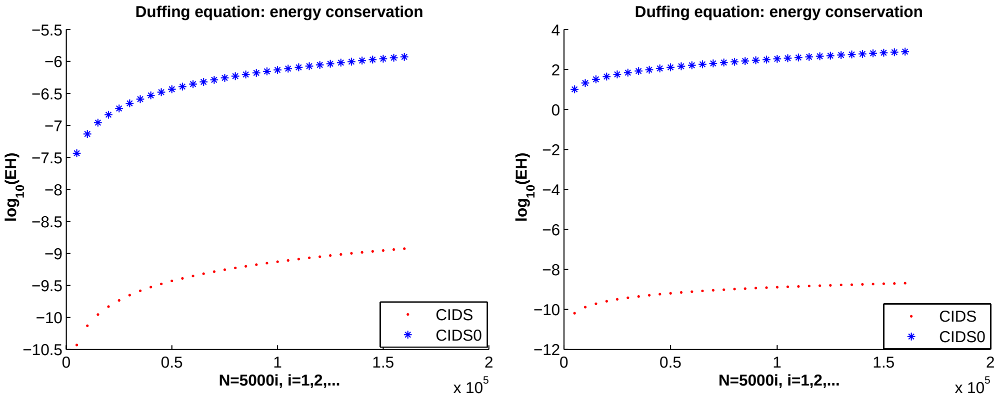
$$q(t) = sn(\omega t, k/\omega),$$

and represents a periodic motion in terms of the Jacobian elliptic function sn. In this test, we choose the parameter values $k = 0.03$, $t_{\mathrm{end}} = 10\,000$.

Since it is a one-dimensional problem, only CIDS and CIDS0 methods are used. First, for the fixed-point iteration at each step, we set the maximum iteration number as 10 and the error tolerance as 10^{-15}. We plot the logarithm of the errors $EH = \max |H(p_{5000i}, q_{5000i}) - H(p_0, q_0)|$ of the Hamiltonian against $N = 5000i$ for $\omega = 10$ and $\omega = 20$ with $h = 1/2^4$. The results are shown in figure 1. Then we set the maximum iteration number as 1000 and apply the two methods to the system with different error tolerance for the fixed-point iteration. We plot the logarithm of the total iteration number against the logarithm of the error tolerance of the iteration for the two methods with $h = 1/2^4$, where the total iteration number means the summation of all the numbers of iterations at each step from the initial time t_0 to the final time t_{end}. The results are shown in figure 2.

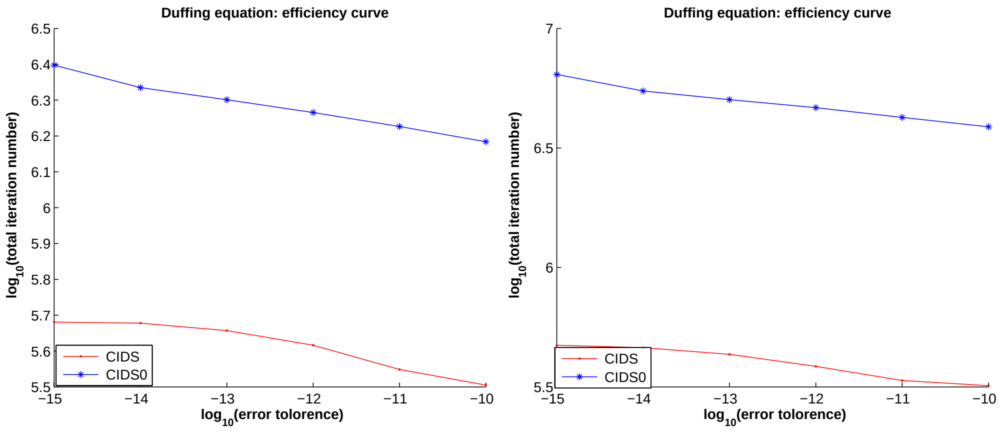
Problem 2. Consider the Fermi–Pasta–Ulam problem (this problem is considered in [1, 18]), which can be expressed by a Hamiltonian system with the Hamiltonian

$$H(p, q) = \tfrac{1}{2}p^T p + \tfrac{1}{2}q^T M q + U(q),$$



$(a)\ \omega = 10,\ h = \frac{1}{2^4}$ $(b)\ \omega = 20,\ h = \frac{1}{2^4}$

Figure 1. Problem 1 (maximum iteration number = 10): the logarithm of the errors of Hamiltonian $EH = |H(p_{5000i}, q_{5000i}) - H(p_0, q_0)|$ against $N = 5000i$, $i = 1, 2, \ldots$.



$(a)\ \omega = 10,\ h = \frac{1}{2^4}$ $(b)\ \omega = 20,\ h = \frac{1}{2^4}$

Figure 2. Problem 1 (maximum iteration number = 1000): the logarithm of the total iteration number against the logarithm of the error tolerance of the iteration.

where

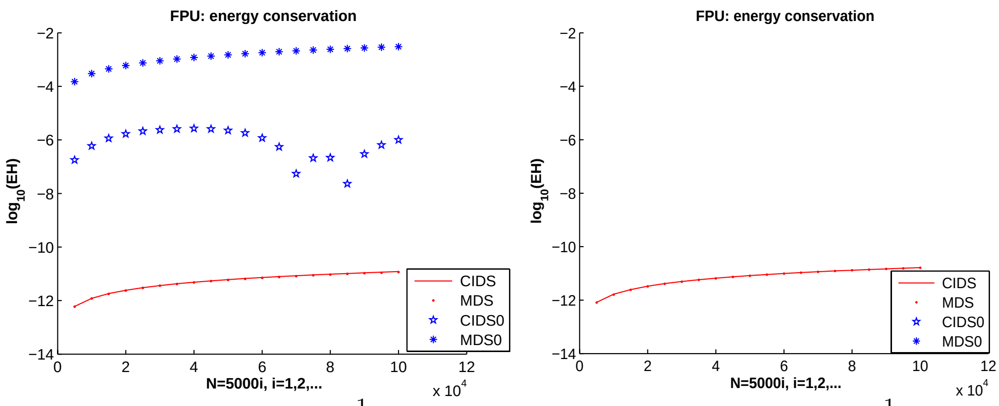
$$M = \begin{pmatrix} \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times m} & \omega^2 I_{m\times m} \end{pmatrix},$$

$$U(q) = \frac{1}{4}\left((q_1 - q_{m+1})^4 + \sum_{i=1}^{m-1}(q_{i+1} - q_{m+i+1} - q_i - q_{m+i})^4 + (q_m + q_{2m})^4\right).$$

Here, q_i represents a scaled displacement of the ith stiff spring, q_{m+i} is a scaled expansion (or compression) of the ith stiff spring, and p_i, p_{m+i} are their velocities (or momenta).

Following [1], we choose

$$m = 3,\ q_1(0) = 1,\ p_1(0) = 1,\ q_4(0) = \frac{1}{\omega},\ p_4(0) = 1, \tag{54}$$



$(a)\ \omega = 100,\ h = \dfrac{1}{100}$ $(b)\ \omega = 200,\ h = \dfrac{1}{100}$

Figure 3. Problem 2 (maximum iteration number $= 10$): the logarithm of the errors of Hamiltonian $EH = |H(p_{5000i}, q_{5000i}) - H(p_0, q_0)|$ against $N = 5000i$.

and choose zero for the remaining initial values. We apply the methods MDS, MDS0, CIDS and CIDS0 to the system. The system with the initial values (54) is integrated in the interval $[0, 1000]$ with the step size $h = 1/100$ for $\omega = 100$ and $\omega = 200$.

First, for the fixed-point iteration at each step, we set the maximum iteration number as 10, the error tolerance as 10^{-15} and plot the logarithm of the errors of Hamiltonian $EH = \max |H(p_{5000i}, q_{5000i}) - H(p_0, q_0)|$ against $N = 5000i$, $i = 1, 2, \ldots$. If the error is very large, we do not plot the points in the figure. The results are shown in figure 3. As we can see from the result, for fixed $h = 1/100$, as ω increases from 100 to 200, the traditional discrete gradient methods are no longer convergent; however, the new schemes still converge well.

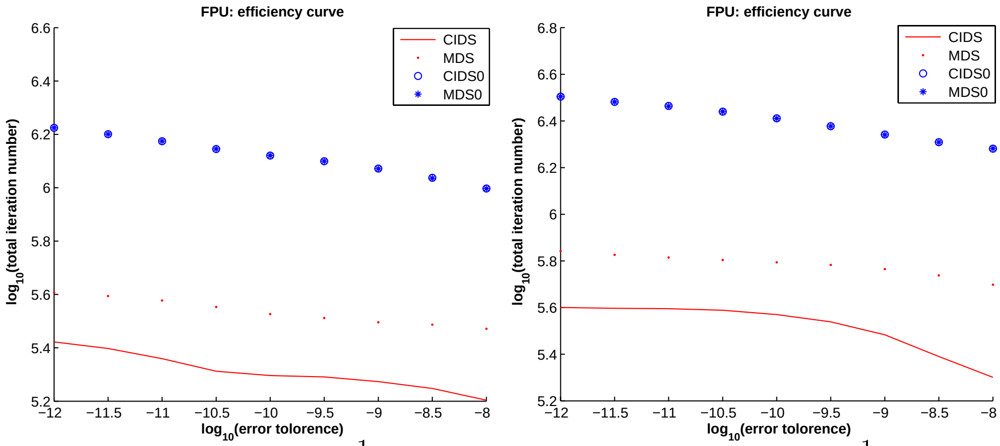
Then we set the maximum iteration number as 1000, and choose $h = 1/100$ for $\omega = 100$, $h = 1/200$ for $\omega = 200$. We plot the logarithm of the total iteration number against the logarithm of the error tolerance of the iteration for the four methods. The results are shown in figure 4.

Problem 3. Consider the sine-Gordon equation with periodic boundary conditions (see [17])

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial^2 u}{\partial x^2} - \sin u, \quad -1 < x < 1, \quad t > 0, \\ u(-1, t) = u(1, t). \end{cases}$$

By semi-discretization on the spatial variable with second-order symmetric differences, and introducing generalized momenta $p = \dot{q}$, we obtain the Hamiltonian system with the Hamiltonian

$$H(p, q) = \tfrac{1}{2} p^T p + \tfrac{1}{2} q^T M q + U(q),$$



(*a*) $\omega = 100,\ h = \dfrac{1}{100}$ (*b*) $\omega = 200,\ h = \dfrac{1}{200}$

Figure 4. Problem 2 (maximum iteration number = 1000): the logarithm of the total iteration number against the logarithm of the error tolerance of the iteration.

where $q(t) = (u_1(t), \ldots, u_d(t))^T$ and $U(q) = -(\cos(u_1) + \cdots + \cos(u_d))$ with $u_i(t) \approx u(x_i, t),\ x_i = -1 + \mathrm{i}\Delta x, i = 1, \ldots, d, \Delta x = 2/d$ and

$$M = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}. \tag{55}$$

We take the initial conditions as

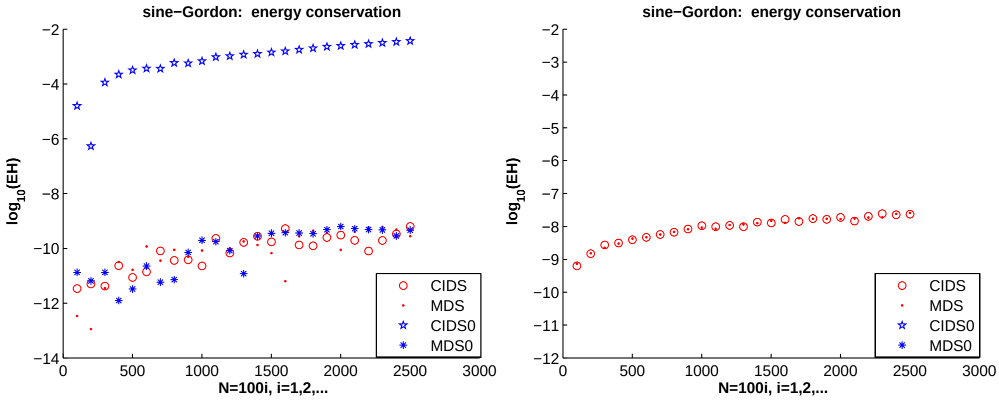
$$q(0) = (\pi)_{i=1}^{d}, \quad p(0) = \sqrt{d}\left(0.01 + \sin\left(\frac{2\pi \mathrm{i}}{d}\right)\right)_{i=1}^{d}.$$

The system is integrated in the interval [0, 100] with the methods MDS, MDS0, CIDS and CIDS0. First, for the fixed-point iteration at each step, we set the maximum iteration number as 10 and the error tolerance as 10^{-15}. We plot the logarithm of the errors of Hamiltonian $EH = \max |H(p_{100i}, q_{100i}) - H(p_0, q_0)|$ against $N = 100i$ for $d = 36$ and $d = 144$ with $h = 0.04$. If the error is very large, we do not plot the points in the figure. The results are shown in figure 5.

Then we set the maximum iteration number as 1000. We apply the four methods to the system in the interval [0, 10] with step size $h = 0.04$ for $d = 36$ and $h = 0.01$ for $d = 144$. We plot the logarithm of the total iteration number against the logarithm of the error tolerance of the iteration for the four methods. The results are shown in figure 6. As we can see from the results, compared with the traditional discrete gradient methods, the fixed-point iteration of the new methods have much larger convergence domain, and the convergence is faster.

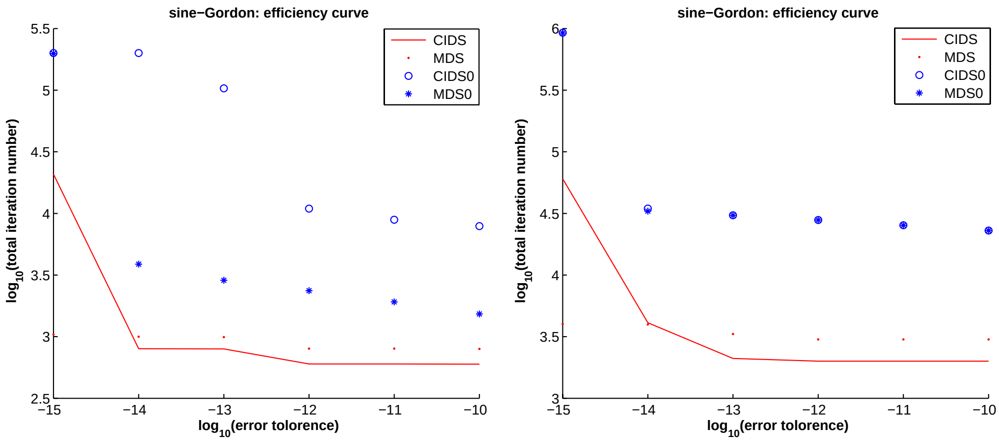
6. Conclusions

In this paper, combining the idea of the discrete gradient method with the ERKN integrator, we derive and analyze a new and extended discrete gradient formula for the oscillatory Hamiltonian



(a) $d = 36,\ h = 0.04$ (b) $d = 144,\ h = 0.04$

Figure 5. Problem 3 (maximum iteration number = 10): the logarithm of the errors of Hamiltonian $EH = |H(p_{100i}, q_{100i}) - H(p_0, q_0)|$ against $N = 100i$, $i = 1, 2, \ldots$.



(a) $d = 36,\ h = 0.04$ (b) $d = 144,\ h = 0.01$

Figure 6. Problem 3 (maximum iteration number = 1000): the logarithm of the total iteration number against the logarithm of the error tolerance of the iteration.

system. Some properties of the new formula are presented. It is the distinguishing feature of the new formula to take advantage of the special structure of the system brought by the linear term Mq, so that the extended discrete gradient methods specially adapt themselves to the oscillatory system. Since both the extended discrete gradient schemes and the traditional ones are implicit, an iterative procedure is required. From the convergence analysis of the fixed-point iteration for the implicit schemes, it can be observed that a larger step size can be chosen for the extended discrete gradient schemes than that for the traditional discrete gradient methods when applied to the oscillatory Hamiltonian systems. The convergence rate of the extended discrete gradient methods is much higher than that of the traditional ones. The results of numerical experiments also clearly support this point. Another very important property is that the convergence of the fixed-point iteration for the extended discrete gradient schemes is independent of M. Unfortunately, however, the convergence of the fixed-point iteration for the traditional discrete gradient methods is dependent on M.

It can be concluded that the new schemes are much more efficient as compared to the traditional discrete gradient methods in the scientific literature.

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