A new symmetric linearly implicit exponential integrator preserving polynomial invariants or Lyapunov functions for conservative or dissipative systems

System

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Abstract

We present a new symmetric linearly implicit exponential integrator that preserves the polynomial first integrals or the Lyapunov functions for the conservative and dissipative stiff equations, respectively. The method is tested by both oscillated ordinary differential equations and partial differential equations, e.g., an averaged system in wind-induced oscillation, the Fermi–Pasta–Ulam systems, and the polynomial pendulum oscillators. The numerical simulations confirm the conservative properties of the proposed method and demonstrate its good behavior in superior running speed when compared with fully implicit schemes for long-time simulations.

Keywords: Linearly implicit, energy-preserving, exponential integrator, conservative system, dissipative system

1. Introduction

This paper focuses on the semilinear systems of the form

$$\dot{y}(t) = Ay + f(y), \quad y(t_0) = y_0,$$
(1)

where A is a linear unbounded differential operator or a matrix which has eigenvalues with large negative real part or with purely imaginary eigenvalues of large modulus, and the non-linear term f is supposed to be nonstiff satisfying Lipschitz condition. The semilinear system (1) arises in many applications, such as the charged-particle dynamic [1], the rapidly rotating shallow water equations for semi-geostrophic particle motion [2], and the semi-discretization of semilinear PDEs. Equation (1) is usually stiff and one popular class of numerical integrators that are suitable for such problems is the exponential integrators [3]. These methods normally permit larger step sizes and provide higher accuracy than the non-exponential integrators. The basic idea behind such methods is to solve the stiff part with an exact solver. Based on the variation of constants formula, the exact solution of (1) is given by

$$y(t_0 + h) = \exp(hA)y_0 + h \int_0^1 \exp((1 - \tau)hA)f(y(t_0 + \tau h))d\tau, \qquad (2)$$

where the integration interval is $[t_0, t_0 + h]$. Most exponential integrators can be obtained from an appropriate approximation of the integral in exact solution (2). For example, the exponential Euler method is obtained by interpolating the nonlinear term at y_0 with the form

$$y_1 = \exp(hA)y_0 + h\phi(hA)f(y_0),$$

and the implicit exponential Euler method is given by interpolating the nonlinear term at y_1 with the form

$$y_1 = \exp(hA)y_0 + h\phi(hA)f(y_1),$$

where $\phi(z) := \frac{e^z - 1}{z}$ [3]. More examples of exponential integrators can be found in, e.g., [3, 4].

Equation (1) might possess important geometric structures. In particular, the canonical Hamiltonian structure corresponds to equations of the form

$$\dot{y}(t) = J\nabla H(y), \quad y(t_0) = y_0, \tag{3}$$

where

$$H(y) = \frac{1}{2}y^T M y + U(y),$$

and

$$J = \begin{bmatrix} 0 & I_m \\ -I_m & 0 \end{bmatrix}$$

with I_m an identity matrix, M a symmetric matrix and U(y) a scalar function. Two prominent features of equation (3) are the conservation of the energy function H(y) and the preservation of the symplecticity. In this work, we intend to focus on more general equations than the canonical Hamiltonian systems, where the matrix J in (3) is allowed to be a constant skewsymmetric matrix or a negative semidefinite matrix. A skew-symmetric matrix J grantees the conservation of the energy, while a negative semidefinite matrix J will lead to a dissipative system with Lyapunov function H(y)monotonically decreasing. In view of these special structures in equation (3), a type of candidate methods will be the structure-preserving exponential integrators which have superior qualitative behavior over long-time integration compared with the general-purpose designed higher-order methods [5]. Examples include symmetric methods [6], symplectic methods [7] and energy-preserving methods [8]. Here we would like to consider particularly energy-preserving exponential integrators. Such methods in previous work are fully implicit, e.g., [8, 9, 10, 11], except for the recent work [12], where a linearly implicit method for the nonlinear Klein–Gordon equation was considered using the scalar auxiliary variable (SAV) [13] approach. For linearly implicit methods, only one linear system is solved in each iteration and thus less computational cost is needed. For this consideration, we expect to construct linearly implicit methods in this work.

There are two mostly used techniques in creating linearly implicit energypreserving methods for general conservative/dissipative systems with gradient flow, according to the authors' best knowledge. The first one follows from Furihata and co-authors, where multiple-point methods are used so that the nonlinearity can be portioned out [14]. Further studies of this method were presented in [15] and [16] using the concept of polarized energy and polarized discrete gradient. The second technique is to combine the linearly implicit Crank-Nicolson method and the invariant energy quadratization (IEQ) [17] or the scalar auxiliary variable (SAV) [13] approach. Both the IEQ-based and the SAV-based methods are applicable for nonlinear systems, including nonpolynomials; however, these methods need bounded free energy regarding the nonlinear terms. Besides, the linearly implicit methods constructed based on the second approach have no symmetric property. This paper will focus on the technique using polarized energy for problems with polynomial energy functions. There are several reasons for choosing this technique. First, there are huge amounts of PDEs and ODEs with polynomial energy functions, e.g., the nonlinear Schrödinger equations, the nonlinear wave equations, the KdV equations, the Camassa-Holm equations, the wind-induced oscillator, the polynomial pendulum oscillator, and so on. Second, there are no other restrictions for the nonlinear terms except for being polynomials. Third, the general scheme of the methods based on the first technique looks much more straightforward than the second technique. Last but not least, the linearly implicit methods constructed based on the first technique can be symmetric, and it has been shown that symmetric methods applied to (near-)integrable reversible systems share similar properties to symplectic methods: linear error growth, long-time near-conservation of first integrals and existence of invariant tori [18]. Thus methods with symmetric property usually provide prominent long-time behavior.

The paper is organized as follows. First, we construct the symmetric linearly implicit energy-preserving exponential integrators and discuss their properties in Section 2. In Section 3, numerical examples are presented to illustrate the performance of the proposed method. In the last section, we conclude the paper with a summary of the properties and advantages shared by the method.

2. Symmetric linearly implicit energy-preserving exponential scheme

In this section, we combine the idea of constructing linearly implicit methods using polarized energy [15] and the idea of constructing energypreserving exponential methods using discrete gradient [8] to build the symmetric linearly implicit energy-preserving exponential integrators. To present the method more intuitively, we restrict the nonlinear term U(y) (potential energy) in equation (3) to be a cubic polynomial. However, the method is also applicable to problems with any higher-order polynomials, for which the results will be introduced briefly in this paper too.

The critical point of using polarized energy to construct a linearly implicit method is to portion out the nonlinearity over consecutive time steps. This can be carried out by constructing quadratic polarized energy and then performing the polarized discrete gradient method, similarly as shown in [19] for a cubic polynomial. A systematical way of constructing a quadratic polarization for higher-order polynomial functions is presented in [15], for example

- $U(x) = x^2$ can be polarized by $\overline{U}(x, y) = \theta \frac{x^2 + y^2}{2} + (1 \theta)xy, \ \theta \in [0, 1],$
- $U(x) = x^3$ can be polarized by $\overline{U}(x, y) = x \frac{x+y}{2}y$,
- $U(x) = x^4$ can be polarized by $\overline{U}(x, y) = x^2 y^2$,
- $U(x) = x^5$ can be polarized by $\overline{U}(x, y, z, w) = xyzw\frac{x+y+z+w}{4}$,

• $U(x) = x^6$ can be polarized by $\overline{U}(x, y, z) = x^2 y^2 z^2$.

Following from [19], $\overline{\nabla}\overline{U}$ is said to be a polarized discrete gradient for a polarized energy \overline{U} if the following conditions hold

$$\bar{U}(y,z) - \bar{U}(x,y) = \frac{1}{2}(z-x)^T \overline{\nabla} \bar{U}(x,y,z),$$

$$\overline{\nabla} \bar{U}(x,x,x) = \nabla U(x).$$
(4)

We will use the polarized discrete gradient to construct the linearly implicit energy-preserving exponential integrators. Consider the variation of constants formula on interval $[t_0, t_0 + 2h]$ for problem (1) in the form

$$y(t_0 + 2h) = \exp(2hJM)y_0 + 2h\int_0^1 \exp(2(1-\xi)hJM)J\nabla U(y(t_0 + 2h\xi))d\xi.$$
(5)

Substituting $\nabla U(y(t_0+2h\xi))$ with the polarized discrete gradient $\overline{\nabla}\overline{U}(y_0, y_1, y_2)$ in (5), we obtain the energy-preserving exponential integrator for problem (3) as follows

$$y_{n+2} = \exp(2hJM)y_n + 2h\phi(2hJM)J\overline{\nabla}\overline{U}(y_n, y_{n+1}, y_{n+2}) \qquad \text{(LIEEP).} \quad (6)$$

Remark 1. Suppose that a quadratic polarization of a higher-order polynomial function $U(y_n)$ has the form $\overline{U}(y_n, \dots, y_{n+i}, \dots, y_{n+p-1})$. Then the generalization of the polarized discrete gradient in (4) can be given by

$$\bar{U}(y_{n+1},\cdots,y_{n+p}) - \bar{U}(y_n,\cdots,y_{n+p-1}) = \frac{1}{p}(y_{n+p} - y_n)^T \overline{\nabla} \bar{U}(y_n,\cdots,y_{n+p}),$$
$$\overline{\nabla} \bar{U}(y_n,\cdots,y_{n+p}) = \nabla U(y_n).$$
(7)

Remark 2. Suppose that the polarized discrete gradient for a higher-order polynomial energy function $U(y_n)$ is given by $\overline{\nabla}\overline{U}(y_n, y_{n+1}, \dots, y_{n+p})$ following from equation (7). Then the linearly implicit energy-preserving exponential integrator for problem (3) can be given by

$$y_{n+p} = exp(phJM)y_n + ph\phi(phJM)J\overline{\nabla}\overline{U}(y_n, y_{n+1}, \cdots, y_{n+p}).$$
(8)

Remark 3. Scheme (6) is a special case of scheme (8) with p = 2.

Before presenting the main theorems about the proposed method's conservative properties, we begin with a lemma. **Lemma 1.** For any symmetric matrix M, positive integer p and scalar h > 0, the matrix

$$B = exp(phJM)^T M exp(phJM) - M$$

is zero when J is skew-symmetric and negative semidefinite when J is negative semidefinite.

The proof of this lemma follows directly from Lemma 2.2 in [8] since the result does not change when h is replaced by ph.

Theorem 1. Scheme (6) preserves the following polarized energy

$$\bar{H}(y_n, y_{n+1}) = \frac{1}{4} (y_n^T M y_n + y_{n+1}^T M y_{n+1}) + \bar{U}(y_n, y_{n+1}).$$
(9)

Proof. We first assume that the matrix M is not singular and denote by $V = 2hJM, M^{-1}\overline{\nabla}\overline{U} = \overline{\nabla}\widetilde{U}$. The energy error has the form

$$\bar{H}(y_{n+1}, y_{n+2}) - \bar{H}(y_n, y_{n+1})
= \frac{1}{4}(y_{n+2}^T M y_{n+2} + y_{n+1}^T M y_{n+1}) - \frac{1}{4}(y_n^T M y_n + y_{n+1}^T M y_{n+1})
+ \bar{U}(y_{n+1}, y_{n+2}) - \bar{U}(y_n, y_{n+1}).$$
(10)

By replacing $y_{n+2} = \exp(V)y_n + 2h\phi(V)J\overline{\nabla}\overline{U}(y_n, y_{n+1}, y_{n+2})$ and using $\phi(V)V = \exp(V) - I$, we get the following equations

$$\frac{1}{4}(y_{n+2}^{T}My_{n+2} + y_{n+1}^{T}My_{n+1}) - \frac{1}{4}(y_{n}^{T}My_{n} + y_{n+1}^{T}My_{n+1}) \\
= \frac{1}{4}y_{n}^{T}(\exp(V)^{T}M\exp(V) - M)y_{n} + hy_{n}^{T}\exp(V)^{T}M\phi(V)J\overline{\nabla}\bar{U} \\
+ h^{2}(\overline{\nabla}\bar{U})^{T}J^{T}\phi(V)^{T}M\phi(V)J\overline{\nabla}\bar{U} \tag{11}$$

$$= \frac{1}{4}y_{n}^{T}(\exp(V)^{T}M\exp(V) - M)y_{n} + \frac{1}{2}y_{n}^{T}\exp(V)^{T}M(\exp(V) - I)\overline{\nabla}\tilde{U} \\
+ \frac{1}{4}(\overline{\nabla}\tilde{U})^{T}(\exp(V) - I)^{T}M(\exp(V) - I)\overline{\nabla}\tilde{U},$$

and

$$U(y_{n+1}, y_{n+2}) - U(y_n, y_{n+1})$$

$$= \frac{(y_{n+2} - y_n)^T}{2} \overline{\nabla} \overline{U}(y_n, y_{n+1}, y_{n+2})$$

$$= \frac{1}{2} y_n^T (\exp(V)^T - I) \overline{\nabla} \overline{U} + h(\overline{\nabla} \overline{U})^T J^T \phi(V)^T \overline{\nabla} \overline{U}$$

$$= \frac{1}{2} y_n^T (\exp(V)^T M - M) \overline{\nabla} \widetilde{U} + \frac{1}{2} \overline{\nabla} \widetilde{U}^T V^T \phi(V)^T M \overline{\nabla} \widetilde{U}$$

$$= \frac{1}{2} y_n^T (\exp(V)^T M - M) \overline{\nabla} \widetilde{U} + \frac{1}{2} \overline{\nabla} \widetilde{U}^T (\exp(V)^T M - M) \overline{\nabla} \widetilde{U}.$$
(12)

Inserting equations (11) and (12) to equation (10), we obtain the following results

$$\begin{split} \bar{H}(y_{n+1}, y_{n+2}) &- \bar{H}(y_n, y_{n+1}) \\ &= \frac{1}{4} y_n^T (\exp(V)^T M \exp(V) - M) y_n + \frac{1}{2} y_n^T (\exp(V)^T M \exp(V) - M) \overline{\nabla} \tilde{U} \\ &+ \frac{1}{4} \overline{\nabla} \tilde{U}^T (\exp(V)^T M \exp(V) - M) \overline{\nabla} \tilde{U} + \frac{1}{4} \overline{\nabla} \tilde{U}^T (\exp(V)^T M - M \exp(V)) \overline{\nabla} \tilde{U} \\ &= \frac{1}{4} (y_n + \overline{\nabla} \tilde{U})^T (\exp(V)^T M \exp(V) - M) (y_n + \overline{\nabla} \tilde{U}) \\ &+ \frac{1}{4} \overline{\nabla} \tilde{U}^T (\exp(V)^T M - M \exp(V)) \overline{\nabla} \tilde{U} \\ &= 0, \end{split}$$
(13)

where the last step follows from the fact that $\exp(V)^T M - M\exp(V)$ is skew-symmetric, and $\exp(V)^T M\exp(V) - M$ is also skew-symmetric from Lemma 1.

For a singular M, one can find a series of non-singular and symmetric matrices M_{ϵ} such that $M_{\epsilon} = M$ when $\epsilon \to 0$. For any M_{ϵ} , we can follow the proof above and show that the polarized energy function in the form

$$\bar{H}_{\epsilon}(y_n^{\epsilon}, y_{n+1}^{\epsilon}) = \frac{1}{4}(y_n^{\epsilon T} M_{\epsilon} y_n^{\epsilon} + y_{n+1}^{\epsilon T} M_{\epsilon} y_{n+1}^{\epsilon}) + \bar{U}(y_n^{\epsilon}, y_{n+1}^{\epsilon})$$

is preserved by the approximation given by

$$y_{n+2}^{\epsilon} = \exp(2hJM_{\epsilon})y_n^{\epsilon} + 2h\phi(2hJM_{\epsilon})J\overline{\nabla}\overline{U}(y_n^{\epsilon}, y_{n+1}^{\epsilon}, y_{n+2}^{\epsilon})$$

for the following problem

$$\dot{y}(t) = JM_{\epsilon}y + J\nabla U(y(t)), \quad y(t_0) = y_0.$$

Therefore, $\bar{H}_{\epsilon}(y_n^{\epsilon}, y_{n+1}^{\epsilon}) = \bar{H}(y_n, y_{n+1})$ is preserved by method (6) when $\epsilon \to 0$.

For problems (3) with higher-order polynomial energy functions, similar conservation property can be obtained by scheme (8), as shown in the following corollary.

Corollary 1. Scheme (8) preserves the following polarized energy

$$\bar{H}(y_n, \cdots y_{n+p-1}) = \frac{1}{2p} \sum_{i=0}^{p-1} y_{n+i}^T M y_{n+i} + \bar{U}(y_n, \cdots, y_{n+p-1}).$$
(14)

The proof is similar to Theorem 1 and thus is omitted here.

Theorem 2. If J is a constant negative semidefinite matrix, scheme (6) preserves the polarized Lyapunov function \overline{H} for problem (3):

$$\bar{H}(y_{n+1}, y_{n+2}) \le \bar{H}(y_{n+1}, y_n),$$

where $\overline{H}(y_n, y_{n+1})$ is defined by equation (9).

Proof. Let us suppose M to be non-singular; otherwise we follow the similar procedure in the proof for Theorem 1, i.e., constructing a series of M_{ϵ} convergent to M to achieve the result.

For a constant negative semidefinite matrix J, the error of Lyapnov function has the same form as the energy error in (13):

$$\begin{split} \bar{H}(y_{n+1}, y_{n+2}) &- \bar{H}(y_n, y_{n+1}) \\ &= \frac{1}{4}(y_{n+2}^T M y_{n+2} + y_{n+1}^T M y_{n+1}) - \frac{1}{4}(y_n^T M y_n + y_{n+1}^T M y_{n+1}) \\ &+ \bar{U}(y_{n+1}, y_{n+2}) - \bar{U}(y_n, y_{n+1}) \\ &= \frac{1}{4}(y_n + \overline{\nabla}\tilde{U})^T (\exp(V)^T M \exp(V) - M)(y_n + \overline{\nabla}\tilde{U}) \\ &+ \frac{1}{4}\overline{\nabla}\tilde{U}^T (\exp(V)^T M - M \exp(V))\overline{\nabla}\tilde{U} \\ &\leq 0, \end{split}$$

where the last step follows from the fact that $\exp(V)^T M - M\exp(V)$ is skewsymmetric, and $\exp(V)^T M\exp(V) - M$ is negative semidefinite according to Lemma 1.

Similarly, for problems (3) with a higher-order polynomial energy, we have the following corollary.

Corollary 2. If J is a constant negative semidefinite matrix, scheme (8) preserves the polarized Lyapunov function:

$$\bar{H}(y_{n+1},\cdots,y_{n+p}) \leq \bar{H}(y_n,\cdots,y_{n+p-1}),$$

where $\overline{H}(y_n, \cdots, y_{n+p-1})$ has the same form as equation (14).

The proof is similar to Theorem 2 and thus is omitted here.

Theorem 3. Scheme (6) is symmetric.

Proof. Exchanging y_n , $y_{n+1} \leftrightarrow y_{n+2}$, y_{n+1} and replacing 2h by -2h in (6), we obtain

$$y_n = \exp(-V)y_{n+2} - 2h\phi(-V)J\overline{\nabla}\overline{U}(y_{n+2}, y_{n+1}, y_n).$$

Following from the definition in (4) and the cyclic permutation free property of the polarized energy [15], we get

$$\overline{\nabla}\overline{U}(y_{n+2}, y_{n+1}, y_n) = \overline{\nabla}\overline{U}(y_n, y_{n+1}, y_{n+2}).$$
(15)

Using $\exp(V)\phi(-V) = \phi(V)$ and the relation in (15), we then obtain

$$y_{n+2} = \exp(V)y_n + 2h\phi(V)J\overline{\nabla}\overline{U}(y_n, y_{n+1}, y_{n+2}).$$

Scheme (8) for problems with higher-order polynomial U(y) also holds the symmetric property if the polarization of the function U(y) is invariant when the order of its arguments is reversed. This can be obtained by symmetrizing over dihedral group [15]. Although only cyclic permutation free is required in the definition of the polarized energy, we can actually always get a permutation free quadratic polarization for any higher order polynomial $\overline{U}(y)$. In fact, the polarization examples shown above are all permutation free. In this paper, we always consider permutation free polarization, i.e., quadratic polarization satisfying the following condition

$$\overline{U}(y_n, \cdots y_{n+p-1}) = \overline{U}(y_{n+i_1-1}, \cdots y_{n+i_p-1}), \quad (i_1, \cdots, i_p) \in S_p,$$

where S_p is a symmetric group.

Corollary 3. Scheme (8) is symmetric if the polarization of function U(y) is permutation free.

The proof is similarly to the proof of Theorem 3 except that the cyclic permutation free property should be replaced by the permutation free property.

3. Numerical experiment

The proposed method is suitable for conservative or dissipative differential equations of the form (3) with J a constant skew-symmetric or negative semidefinite matrix and U(y) a scalar polynomial function of any order. These equations include the highly oscillatory conservative or dissipative ODEs and also the semi-discrete systems arising from PDEs. In this section, we test our method by three differential equations. The first two examples are used to demonstrate the efficient behavior of the method compared to the fully implicit method, e.g., the energy-preserving exponential integrators based on the averaged vector field method, denoted by EAVF. The third example is chosen to show the application of the method for problems with higher-order polynomial energy functions.

EAVF method was put forward in [8], which has the form

$$y_{n+1} = \exp(hJM)y_n + h\phi(hJM)J\overline{\nabla}U(y_n, y_{n+1}), \tag{16}$$

where $\overline{\nabla}U(y_n, y_{n+1}) = \int_0^1 \nabla U((1-\tau)y_n + \tau y_{n+1})d\tau$. Besides, scheme (16) has been shown to preserve the discrete energy of the form

$$H(y_n) = \frac{1}{2} y_n^T M y_n + U(y_n).$$
 (17)

The integral in EAVF method is evaluated by the 2-point GL quadrature formula, which gives an exact approximation of the integration. In most cases, the terms $\exp(phJM)$ and $\phi(phJM)$ (*p* is a positive integer number) can not be calculated explicitly, and we use the MATLAB package proposed in [20] to compute them, where Pade approximations are used.

In the experiments, the global error is defined by

$$\max_{n\geq 0} \|y_n - y(t_n)\|,$$

where $t_n = t_0 + nh$ with h the time step size, and $y(t_n)$ is the reference exact solution. In this work, we compute the reference solution by the 6-order continuous Runge–Kutta (CRK) method [21] with the form

$$\begin{cases} y_{n+1/3} = y_n + hJ \int_0^1 \left(\frac{37}{27} - \frac{32}{9}\sigma + \frac{20}{9}\sigma^2\right) \nabla H(Y_\sigma) d\sigma \\ y_{n+2/3} = y_n + hJ \int_0^1 \left(\frac{26}{27} + \frac{8}{9}\sigma - \frac{20}{9}\sigma^2\right) \nabla H(Y_\sigma) d\sigma \\ y_{n+1} = y_n + hJ \int_0^1 \nabla H(Y_\sigma) d\sigma \end{cases},$$

where

$$Y_{\sigma} = -\frac{(3\sigma - 1)(3\sigma - 2)(\sigma - 1)}{2}y_n + \frac{3\sigma(3\sigma - 2)(3\sigma - 3)}{2}y_{n+1/3} - \frac{3\sigma(3\sigma - 1)(3\sigma - 3)}{2}y_{n+2/3} + \frac{\sigma(3\sigma - 1)(3\sigma - 2)}{2}y_{n+1},$$

and the integrals are evaluated exactly by the 5-point GL quadrature. For all fully implicit schemes, we solve the nonlinear system by the fixed point iteration with tolerance as 10^{-14} . All the numerical results presented are obtained from schemes implemented in MATLAB (2020a release), running on a MacBook Pro with a dual-core 2.6 GHz Intel 6-Core i7 processor and 16 GB of 2667 MHz DDR4 RAM.

Test problem one. We consider an averaged system in wind-induced oscillation [22]

$$\dot{x}_1 = -\zeta x_1 - \lambda x_2 + x_1 x_2,$$

$$\dot{x}_2 = \lambda x_1 - \zeta x_2 + \frac{1}{2} (x_1^2 - x_2^2),$$
(18)

where $\zeta \geq 0$ is a damping factor and λ is a detuning parameter with $\zeta = r\cos(\theta), \ \lambda = r\sin(\theta), \ r \geq 0, \ 0 \leq \theta \leq \pi/2$. Equation (18) can be rewritten into the form (3) with

$$J = \begin{bmatrix} -\cos(\theta) & -\sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{bmatrix} \quad M = \begin{bmatrix} r & 0 \\ 0 & r \end{bmatrix},$$

$$U = -\frac{1}{2}sin(\theta)(x_1x_2^2 - \frac{1}{3}x_1^3) + \frac{1}{2}cos(\theta)(\frac{1}{3}x_2^3 - x_1^2x_2)$$

Its energy function (when $\theta = \pi/2$) or Lyapunov function (dissipative case, when $\theta \leq \pi/2$) is

$$H = \frac{1}{2}r(x_1^2 + x_2^2) - \frac{1}{2}sin(\theta)(x_1x_2^2 - \frac{1}{3}x_1^3) + \frac{1}{2}cos(\theta)(\frac{1}{3}x_2^3 - x_1^2x_2).$$

The matrix exponential in scheme (6) for problem (18) can be calculated explicitly as follows

$$exp(V) = \begin{bmatrix} exp(-2hcr)cos(2hsr) & -exp(-2hcr)sin(2hsr) \\ exp(-2hcr)sin(2hsr) & exp(-2hcr)cos(2hsr) \end{bmatrix},$$

with $c = cos(\theta)$ and $s = sin(\theta)$. We can obtain a polarized discrete gradient $\nabla \overline{U}(x^n, x^{n+1}, x^{n+2})$ based on a polarization of U given by

$$\bar{U}(x^{n}, x^{n+1}) = -\frac{1}{2}sin(\theta) \left(a\frac{x_{1}^{n} + x_{1}^{n+1}}{2}x_{2}^{n}x_{2}^{n+1} + (1-a)\frac{x_{1}^{n}(x_{2}^{n+1})^{2} + x_{1}^{n+1}(x_{2}^{n})^{2}}{2} - \frac{1}{3}x_{1}^{n}\frac{x_{1}^{n} + x_{1}^{n+1}}{2}x_{1}^{n+1}\right) + \frac{1}{2}cos(\theta) \left(\frac{1}{3}x_{2}^{n}\frac{x_{2}^{n} + x_{2}^{n+1}}{2}x_{2}^{n+1} - ax_{1}^{n}x_{1}^{n+1}\frac{x_{2}^{n} + x_{2}^{n+1}}{2} - (1-a)\frac{x_{2}^{n}(x_{1}^{n+1})^{2} + x_{2}^{n+1}(x_{1}^{n})^{2}}{2}\right).$$
(19)

Then we get the linearly implicit energy-preserving scheme in the form of (6) and the polarized energy in the form of (9).

Consider the initial vector $x_1(0) = 0$, $x_2(0) = 1$, r = 20, step size h = 1/20, and the parameters $\theta = \pi/2$ or $\theta = \pi/2 - 10^{-4}$. For LIEEP method, the starting point $[x_1^1, x_2^1]$ is computed by the Matlab function *ode45*. $\theta = \pi/2$ provides a conservative system, and Figure 1a confirms that EAVF method preserves the discrete energy (17) and LIEEP method preserves the polarized energy (9). While $\theta = \pi/2 - 10^{-4}$ leads to a dissipative system, and Figure 1b shows that EAVF method and LIEEP method preserves the discrete of the Lyapunov function in (17) and (9), respectively.

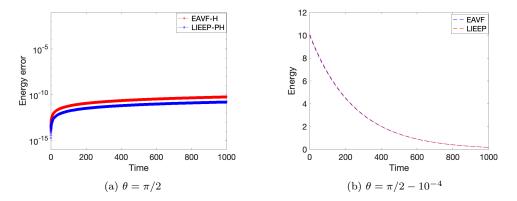


Figure 1: The energy behaviour of both EAVF and LIEEP method with time step size h = 1/20.

In Figure 2 and 3, we consider the global errors and the computational cost using step sizes $h = 1/10/2^i$, with $i = 0, 1, \dots, 5$. Surprisingly, Figure 2a shows that LIEEP method is superconvergent for the conservative system $(\theta = \pi/2)$. We find that this behavior is closely related to the parameter a in the polarized potential energy in (19). We have tried a = 0, 1/2, 1/4, 1, but only a = 1/2 gives a three-order behaviour. Figure 2b shows that the proposed method is more efficient than the fully implicit EAVF method. When $\theta = \pi/2 - 10^{-4}$, i.e., the system is dissipative, the superconvergent behavior disappears for LIEEP method, see Figure 3a. From this figure, we observe that LIEEP method has a convergent issue when the step size is h = 1/10, but with the decrease of the time step size, LIEEP method gets convergent and behaves even better than EAVF method. Figure 3b indicates that the proposed method is much more efficient than EAVF method for the dissipative system.

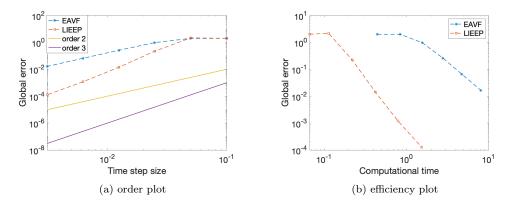


Figure 2: $T = 1000, \ \theta = \pi/2$, the time step sizes are $h = 1/10/2^i$, for $i = 0, 1, \dots, 5$.

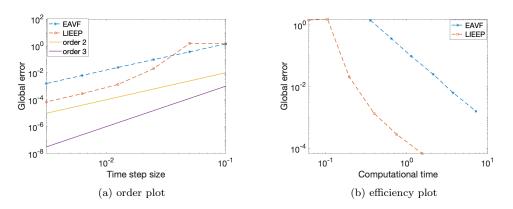


Figure 3: $T = 1000, \theta = \pi/2 - 10^{-4}$, the time step sizes are $h = 1/10/2^i$, for $i = 0, 1, \dots, 5$.

Test problem two. We consider a continuous generalization of an α -FPU (Fermi-Pasta-Ulam) system [23]:

$$\frac{\partial^2 u}{\partial t^2} = \beta \frac{\partial^3 u}{\partial t \partial x^2} + \frac{\partial^2 u}{\partial x^2} (1 + \epsilon (\frac{\partial u}{\partial x})^p) - \gamma \frac{\partial u}{\partial t} - m^2 u, \qquad (20)$$

where $\epsilon > 0$, $\beta \ge 0$ is the coefficient of the internal damping, $\gamma \ge 0$ is the coefficient of the external damping, and $(x,t) \in [0,L] \times [0,T]$. Taking $\frac{\partial u}{\partial t} = v$, equation (20) can be rewritten as

$$\partial_t u = v$$

$$\partial_t v = \beta \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 u}{\partial x^2} (1 + \epsilon (\frac{\partial u}{\partial x})^p) - \gamma v - m^2 u.$$
(21)

Denoting by $y = [u, v]^T$, equation (21) can be reformulated as the following Hamiltonian form

$$\frac{\partial y}{\partial t} = \mathcal{Q}\frac{\delta \mathcal{H}}{\delta y},$$

where

$$\mathcal{Q} = \begin{bmatrix} 0 & 1 \\ -1 & \beta \partial_x^2 - \gamma \end{bmatrix}, \quad \mathcal{H} = \int_0^L E(t, u, v, u_x) dx,$$

with

$$E(t, u, v, u_x) = \frac{1}{2}u_x^2 + \frac{m^2}{2}u^2 + \frac{1}{2}v^2 + \frac{u_x^{p+2}}{(p+2)(p+1)}$$

The function $E(t, u, v, u_x)$ physically represents the local energy density of system (20) at any time t.

Consider p = 1 and the homogeneous Dirichlet boundary conditions u(0,t) = u(L,t) = 0. Discretizing ∂_x^2 with the central difference operator and ∂_x with the forward difference operator, we obtain the following semidiscrete ODE system

$$\dot{y} = Q(My + \nabla U(y)),$$

where

$$Q = \begin{bmatrix} 0 & I \\ -I & \beta D - \gamma I \end{bmatrix}, \quad M = \begin{bmatrix} m^2 I - D & 0 \\ 0 & I \end{bmatrix}, \quad U(y) = \sum_{j=0}^{N-1} \frac{\epsilon}{6} \left(\frac{u_{j+1} - u_j}{\Delta x}\right)^3.$$

Setting $w_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta x}$, and defining the polarized energy

$$\bar{U}(w_j^n, w_j^{n+1}) = \sum_{j=0}^{N-1} \frac{\epsilon}{6} w_j^n \frac{w_j^n + w_j^{n+1}}{2} w_j^{n+1},$$

we can obtain the polarized discrete gradient

$$\bar{\nabla}\bar{U}(w_j^n, w_j^{n+1}, w_j^{n+2}) = \frac{\epsilon}{6\Delta x} w_{j-1}^{n+1}(w_{j-1}^n + w_{j-1}^{n+1} + w_{j-1}^{n+2}) - \frac{\epsilon}{6\Delta x} w_j^{n+1}(w_j^n + w_j^{n+1} + w_j^{n+2}),$$

and the discrete gradient

$$\bar{\nabla}U(w_j^n) = \frac{\epsilon}{2\Delta x} (w_{j-1}^n)^2 - \frac{\epsilon}{2\Delta x} (w_j^n)^2.$$

We consider m = 0, $\epsilon = \frac{3}{4}$, L = 128, T = 100 and spatial step size $\Delta x = 1$. The initial conditions are set to be $u_j(0) = q_j(0)$, $v_j(0) = \dot{q}_j(0)$ and

$$q_j(t) = 5\ln\frac{1 + \exp(2(\alpha(j-97) + t\sinh(\alpha)))}{1 + \exp(2(\alpha(j-96) + t\sinh(\alpha)))} + 5\ln\frac{1 + \exp(2(\alpha(j-32) + t\sinh(\alpha)))}{1 + \exp(2(\alpha(j-33) + t\sinh(\alpha)))}$$

where $\alpha = 0.1$. For LIEEP method, the starting point y_1 is computed by the 6-order CRK method.

In Figure 4a, we fix the external damping coefficient to be zero ($\gamma = 0$) and present the energy behavior of LIEEP method for systems with different internal damping coefficients and a long simulation time T = 500. We observe that the numerical method preserves the energy when there is no damping ($\beta = 0$) and also preserves the dissipation property when the internal damping coefficient is greater than zero, consistent with what is observed in [23], where a fully implicit four-step method is considered. Similar behavior is observed in Figure 4b, where the internal damping coefficient is set to be zero ($\beta = 0$). Figure 5 and 6 confirm that both EAVF and LIEEP method are of order 2 in time, and the comparison of the computational cost between these two methods gives a clear evidence that the proposed method is more efficient than EAVF method. In this experiment, we also present the numerical solutions given by LIEEP method for systems with different settings of β and γ , see Figure 7. These figures clearly demonstrate the dissipative nature of the external damping coefficient, see the change of the colors between Figure 7a and Figure 7b, and the internal damping coefficient, see the change of the shapes between Figure 7a and Figure 7c. These observations in the numerical solutions are in accordance with the results shown by the fully implicit four-step method in [23].

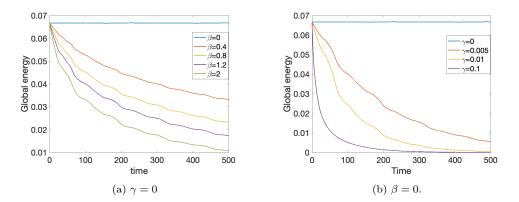


Figure 4: Polarized energy by LIEEP method for α -FPU system with different settings of internal and external damping coefficients. T = 500 and time step size h = 0.025.

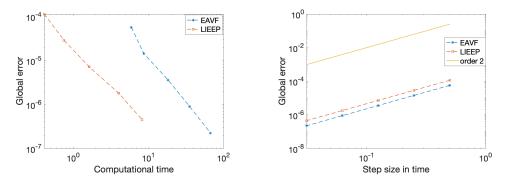


Figure 5: T = 100, $\gamma = 0.005$, $\beta = 0$ and time step size $h = \frac{1}{2^i}$, $i = 1, \dots, 5$, Left: efficiency comparison; right: order plot.

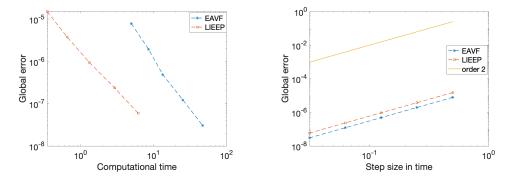


Figure 6: T = 100, $\gamma = 0$, $\beta = 2$ and time step size $h = \frac{1}{2^i}$, $i = 1, \dots, 5$. Left: efficiency comparison; right: order plot.

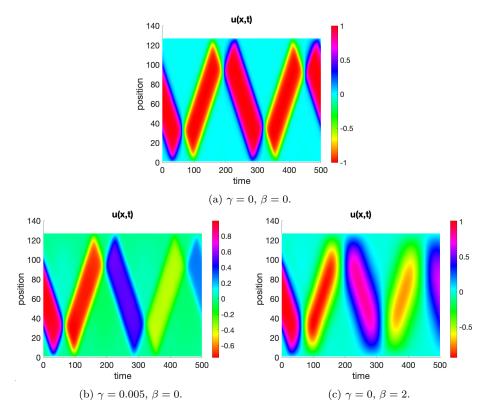


Figure 7: The numerical solution of the α -FPU system with different settings of internal and external damping coefficients on time interval [0, 500] and with time step size h = 0.025.

Test problem three. We consider the polynomial pendulum oscillator, and the main focus of this example is to illustrate the energy conservation property shown in Corollary 1 for the proposed method in Remark 2. Consider the nonlinear pendulum problem with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + 1 - \cos q$$

and a truncated Taylor expansion of the cosine function:

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{24}q^4 + \frac{1}{720}q^6.$$
 (22)

The approximation in (22) to the original problem will be more accurate if even higher-order polynomial is used and |q| is sufficiently small, e.g., $|q| < \frac{1}{2}$ [24]. Denoting by y = [q; p], the polynomial pendulum oscillator with energy function (22) can be rewritten into form (3) with m = 2, J the canonical skew-symmetric matrix, M the identity matrix and

$$U(y) = -\frac{1}{24}q^4 + \frac{1}{720}q^6.$$
 (23)

Consider a polarization of (23) as follows

$$\bar{U}(y_n, y_{n+1}, y_{n+2}) = -\frac{1}{24}q_n q_{n+1} q_{n+2} \frac{q_n + q_{n+1} + q_{n+2}}{3} + \frac{1}{720}q_n^2 q_{n+1}^2 q_{n+2}^2.$$
(24)

We can obtain a polarized discrete gradient of the form

$$\bar{\nabla}\bar{U}(y_n, y_{n+1}, y_{n+2}, y_{n+3}) = \frac{1}{240} q_{n+1}^2 q_{n+2}^2 (q_n + q_{n+3}) - \frac{1}{24} q_{n+1} q_{n+2} (q_n + q_{n+1} + q_{n+2} + q_{n+3}).$$

Take the initial value as $q_0 = 0.5$, $p_0 = 1$ and the integration interval as [0, 1000]. We compute the first two starting points y_1 and y_2 by Matlab function *ode15s*. The polarized energy is reported in Figure 8a, and we observe that it is exactly preserved by LIEEP method defined by equation (8). In this figure, we also present the original discrete energy by LIEEP method, i.e.,

$$H(p_n, q_n) = \frac{1}{2}p_n^2 + 1 - \cos q_n.$$
 (25)

Although LIEEP method does not preserve the exact original energy, Figure 8a shows that the discrete energy given by LIEEP method in the form of (25) stays oscillated and bounded over a long-time integration. Besides, we observe that the numerical solution by LIEEP method applied to the truncated equation provides an approximation with a similar behaviour as the exact solution of the nonlinear pendulum oscillator if a small time step size is considered, e.g., h=0.3, i.e., the phase space is a cylinder, as illustrated in Figure 8b.

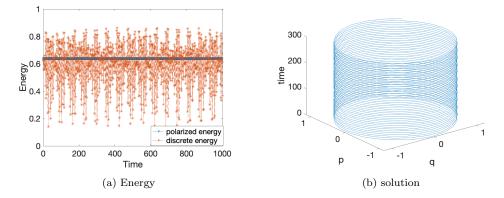


Figure 8: In 8a, the time step size is h = 1, the polarized energy is defined by equation (14) with p = 3 and $\overline{U}(y_n, y_{n+1}, y_{n+2})$ defined by (24); the discrete energy is defined by equation (25). In 8b, the time step size is h = 0.3.

4. Conclusion

This paper constructs a novel symmetric linearly implicit exponential integrator that holds the conservative properties for semi-linear problems with polynomial energy functions. The method is developed based on combining the idea of using polarized discrete gradient to build linearly implicit methods and the idea of using discrete gradient to create energy-preserving exponential integrators. Besides conservative properties, the method is shown to be symmetric, which guarantees excellent long-time behavior.

We test our methods on three types of differential equations, including an oscillated ODE, i.e., the averaged wind-induced oscillator, an oscillated PDE, i.e., the damped FPU problem, and also an ODE with higher-order polynomial energy function, i.e., the polynomial pendulum oscillator. The numerical experiments confirm that the proposed method preserves the polarized energy or the Lyapunov function, and the method is of order two. Moreover, it has been shown that the proposed method has superconvergent behavior for some particular systems when a proper polarized energy is considered. Compared with the fully implicit method (EVAF), our method shows a significantly lower computational cost. In view of the nice properties and the good behavior, we recommend the proposed method for problems with polynomial energy function.

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