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# EXPONENTIAL INTEGRATORS PRESERVING FIRST INTEGRALS OR LYAPUNOV FUNCTIONS FOR CONSERVATIVE OR DISSIPATIVE SYSTEMS*

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**Abstract.** In this paper, combining the ideas of exponential integrators and discrete gradients, we propose and analyze a new structure-preserving exponential scheme for the conservative or dissipative system $\dot{y} = Q(My + \nabla U(y))$, where $Q$ is a $d \times d$ skew-symmetric or negative semidefinite real matrix, $M$ is a $d \times d$ symmetric real matrix, and $U : \mathbb{R}^d \to \mathbb{R}$ is a differentiable function. We present two properties of the new scheme. The paper is accompanied by numerical results that demonstrate the remarkable superiority of our new scheme in comparison with other structure-preserving schemes in the scientific literature.

**Key words.** first integral, Lyapunov function, variation-of-constants formula, exponential integrator, discrete gradient, structure-preserving algorithm

**AMS subject classifications.** 65L04, 65L05, 65M20, 65P10, 65Z05

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## 1. Introduction.

The IVP

$$\dot{y(t)} = Ay(t) + f(y(t)), \quad y(t_0) = y^0, \tag{1}$$

arises most frequently in a variety of applications such as mechanics, molecular dynamics, quantum physics, circuit simulations, and engineering, where $f : \mathbb{R}^d \to \mathbb{R}^d$ and $\cdot$ denotes the derivative operator $\frac{d}{dt}$. An algorithm for (1) is an exponential integrator if it involves the computation of matrix exponentials (or related matrix functions) and integrates the linear system

$$\dot{y(t)} - Ay(t) = 0$$

exactly. In general, exponential integrators permit larger step sizes and achieve higher accuracy than nonexponential ones when (1) is a very stiff differential equation such as highly oscillatory ODEs and semidiscrete time-dependent PDEs. Therefore, numerous exponential algorithms have been proposed for first-order (see, e.g., [1, 10, 20, 22, 23, 24, 25, 26, 30]) and second-order (see, e.g., [11, 12, 14, 18, 33]) ODEs. On the other hand, (1) might inherit many important geometrical/physical structures. For example, the canonical Hamiltonian system

$$\dot{y(t)} = J^{-1}\nabla H(y(t)), \quad y(t_0) = y^0, \tag{2}$$

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is a special case of (1), with

$$J = \begin{pmatrix} O_{d_1 \times d_1} & I_{d_1 \times d_1} \\ -I_{d_1 \times d_1} & O_{d_1 \times d_1} \end{pmatrix}.$$

And the flow of (2) preserves the symplectic 2-form $dy \wedge Jdy$ and the function $H(y)$. In the sense of geometric integration, it is a natural idea to design numerical schemes that preserve the two structures. As far as we know, most research papers dealing with exponential integrators up to now focus on the construction of high-order explicit schemes and fail to be structure preserving except for symmetric/symplectic/energy-preserving methods for first-order ODEs in [5, 7] and oscillatory second-order ODEs (see, e.g., [18, 31, 32]). To combine ideas of exponential integrators and energy-preserving methods, we address ourselves to the system

$$\dot{y} = Q(My + \nabla U(y)), \quad y(t_0) = y^0, \tag{3}$$

where $Q$ is a $d \times d$ real matrix, $M$ is a $d \times d$ symmetric real matrix, and $U : \mathbb{R}^d \to \mathbb{R}$ is a differentiable function. Clearly, (3) could be considered as a special class of (1) or the generalization of (2). However, (3) can exhibit further important structures which should be respected by a structure-preserving scheme. Since $M$ is symmetric, $My + \nabla U(y)$ is the gradient of the function $H(y) = \frac{1}{2} y^{\intercal} My + U(y)$. If $Q$ is skew symmetric, then (3) is a conservative system with the first integral $H$, i.e., $H(y(t))$ is constant; if $Q$ is negative semidefinite (denoted by $Q \leq 0$), then (3) is a dissipative system with the Lyapunov function $H$, i.e., $H(y(t))$ is monotonically decreasing. In these two cases, $H$ is also called the "energy." It should be noted that the choice for $A$ in (1) or $M$ in (3) is not unique. Generally speaking, exponential integrators deal with systems having a major linear term and a comparably small nonlinear term, i.e., $\|A\| \gg \|\frac{\partial f}{\partial y}\|$. Thus, in order to take advantage of exponential integrators, the matrix $M$ in (3) should be chosen such that $\|QM\| \gg \|QHess(U)\|$, where $Hess(U)$ is the Hessian matrix of $U$. For example, highly oscillatory Hamiltonian systems can be characterized by (3) with a dominant linear part, where $M$ implicitly contains the large frequency component. Up to now, many energy-preserving or energy-decaying methods have been proposed in the case of $M = 0$ (see, e.g., [3, 4, 15, 17, 19, 29]). However, these general-purpose methods are not suitable for dealing with (3) when $\|QM\|$ is very large. For one thing, numerical solutions generated by them are far from accurate. For another, they are generally implicit and iterative solutions are required at each step. But the fixed-point iterations for them are not convergent unless the step size is tiny enough. As mentioned at the beginning, these two obstacles are expected to be overcome by introducing exponential integrators. In [31], the authors proposed an energy-preserving adapted average vector field (AAVF) integrator (a trigonometric method) dealing with the second-order Hamiltonian system

$$\begin{cases} \ddot{q}(t) + \tilde{M} q(t) = \nabla V(q(t)), \quad \tilde{M} \text{ is a symmetric matrix}, \\ q(t_0) = q_0, \quad \dot{q}(t_0) = \dot{q}_0, \end{cases}$$

which falls into the class of (3) by introducing $\dot{q} = p$. In this paper, we present and analyze a new exponential integrator for (3) which can preserve the first integral or the Lyapunov function.

The plan of this paper is as follows. In section 2, we construct a general structure-preserving scheme for (3). In section 3, we discuss two important properties of the scheme. Then we present a list of problems which can be solved by this scheme in section 4. Numerical results including the comparison between our new scheme and other structure-preserving schemes in the literature are shown in section 5. The last section is concerned with the conclusion.

## 2. Construction of the structure-preserving scheme for conservative and dissipative systems.

PRELIMINARIES 2.1. *Throughout this paper, given a holomorphic function $f$ in the neighborhood of zero ($f(0) := \lim_{z\to 0} f(z)$ if $0$ is a removable singularity),*

$$f(z) = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} z^i,$$

*and a matrix $A$, the matrix-valued function $f(A)$ being defined by*

$$f(A) = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} A^i.$$

*$I$ and $O$ always denote identity and zero matrices of appropriate dimensions, respectively. $A^{\frac{1}{2}}$ is a square root (not necessarily principal) of a symmetric matrix $A$. If $f^{(i)}(0) = 0$ for odd $i$, then $f(A^{\frac{1}{2}})$ is well-defined for every symmetric $A$ (independent of the choice of $A^{\frac{1}{2}}$). Readers are referred to* [21] *for details about functions of matrices.*

It is well known that the discrete gradient (DG) method is a popular tool for constructing energy-preserving schemes. Broadly speaking, $\overline{\nabla} H(y, \hat{y})$ is said to be a DG of function $H$ if

$$\begin{cases} \overline{\nabla} H(y, \hat{y})^\intercal (y - \hat{y}) = H(y) - H(\hat{y}), \\ \overline{\nabla} H(y, y) = \nabla H(y). \end{cases} \tag{4}$$

Accordingly,

$$y^1 = y^0 + hJ^{-1}\overline{\nabla} H(y^1, y^0) \tag{5}$$

is called a DG method for the system (2). Multiplying $\overline{\nabla} H(y^1, y^0)^\intercal$ on both sides of (5) and using the first identity of (4), we obtain $H(y^1) = H(y^0)$, i.e., the scheme (5) is energy preserving. For more details on the DG method, readers are referred to [15, 28].

On the other hand, most exponential integrators can be derived from the variation-of-constants formula for the problem (3):

$$y(t_0 + h) = \exp(hQM)y(t_0) + h\int_0^1 \exp((1-\xi)hQM)Q\nabla U(y(t_0 + \xi h))d\xi. \tag{6}$$

Replacing $\nabla U(y(t_0 + \xi h))$ with the DG $\overline{\nabla} U(y^1, y^0)$, the integral in (6) can be approx-

imated by:

$$\int_0^1 \exp((1-\xi)hQM)Q\nabla U(y(t_0+\xi h))d\xi$$
$$\approx \left(\int_0^1 \exp((1-\xi)hQM)d\xi\right) Q\overline{\nabla}U(y^1,y^0) = \varphi(hQM)Q\overline{\nabla}U(y^1,y^0),$$

where the scalar function is given by

$$\varphi(z) = (\exp(z)-1)/z.$$

Then we obtain the new scheme

$$y^1 = \exp(V)y^0 + h\varphi(V)Q\overline{\nabla}U(y^1,y^0), \tag{7}$$

where $V = hQM$ and $y^1 \approx y(t_0+h)$.

Due to the energy-preserving property of the DG method, we are hopeful of preserving the first integral by (7) when $Q$ is skew. For convenience, we denote $\overline{\nabla}U(y^1,y^0)$ by $\overline{\nabla}U$ sometimes. To begin with, we give the following preliminary lemma.

LEMMA 2.2. *For any symmetric matrix $M$ and scalar $h \geq 0$, the matrix*

$$B = \exp(hQM)^\intercal M \exp(hQM) - M$$

*satisfies*

$$B = \begin{cases} = 0 & \text{if } Q \text{ is skew symmetric,} \\ \leq 0 & \text{if } Q \leq 0. \end{cases}$$

*Proof.* Consider the linear ODE

$$\dot{y}(t) = QMy(t). \tag{8}$$

When $Q$ is skew, (8) is a conservative equation with the first integral $\frac{1}{2}y^\intercal My$, and its exact solution starting from the initial value $y(0) = y^0$ is $y(t) = \exp(tQM)y^0$. From $\frac{1}{2}y(h)^\intercal My(h) = \frac{1}{2}y^{0\intercal}My^0$, we have

$$\frac{1}{2}y^{0\intercal}\exp(hQM)^\intercal M\exp(hQM)y^0 = \frac{1}{2}y^{0\intercal}My^0$$

for any vector $y^0$. Therefore, $B = \exp(hQM)^\intercal M\exp(hQM) - M$ is skew symmetric. Since it is also symmetric, $B = 0$. The case that $Q \leq 0$ can be proved in a similar way. ∎

THEOREM 2.3. *If $Q$ is skew symmetric, then the scheme* (7) *preserves the first integral $H$ in* (3) *exactly:*

$$H(y^0) = H(y^1),$$

*where $H(y) = \frac{1}{2}y^\intercal My + U(y)$.*

*Proof.* Here we first assume that the matrix $M$ is not singular. We next calculate $\frac{1}{2}y^{1\intercal}My^1$. Let $M^{-1}\overline{\nabla}U=\widetilde{\nabla}U$. Replacing $y^1$ by $\exp(V)y^0+h\varphi(V)Q\overline{\nabla}U(y^1,y^0)$ leads to

$$
\begin{aligned}
&\frac{1}{2}y^{1\intercal}My^1\\
&\quad=\frac{1}{2}(y^{0\intercal}\exp(V)^\intercal+h\overline{\nabla}U^\intercal Q^\intercal\varphi(V)^\intercal)M(\exp(V)y^0+h\varphi(V)Q\overline{\nabla}U)\\
&\quad=\frac{1}{2}y^{0\intercal}\exp(V)^\intercal M\exp(V)y^0+hy^{0\intercal}\exp(V)^\intercal M\varphi(V)Q\overline{\nabla}U\\
&\qquad+\frac{h^2}{2}\overline{\nabla}U^\intercal Q^\intercal\varphi(V)^\intercal M\varphi(V)Q\overline{\nabla}U\\
&\quad=\frac{1}{2}y^{0\intercal}\exp(V)^\intercal M\exp(V)y^0+y^{0\intercal}\exp(V)^\intercal M\varphi(V)V\widetilde{\nabla}U\\
&\qquad+\frac{1}{2}\widetilde{\nabla}U^\intercal V^\intercal\varphi(V)^\intercal M\varphi(V)V\widetilde{\nabla}U\quad(\text{using } V=hQM)\\
&\quad=\frac{1}{2}y^{0\intercal}\exp(V)^\intercal M\exp(V)y^0+y^{0\intercal}\exp(V)^\intercal M(\exp(V)-I)\widetilde{\nabla}U\\
&\qquad+\frac{1}{2}\widetilde{\nabla}U^\intercal(\exp(V)^\intercal-I)M(\exp(V)-I)\widetilde{\nabla}U\quad(\text{using } \varphi(V)V=\exp(V)-I)\\
&\quad=\frac{1}{2}y^{0\intercal}\exp(V)^\intercal M\exp(V)y^0+y^{0\intercal}(\exp(V)^\intercal M\exp(V)-\exp(V)^\intercal M)\widetilde{\nabla}U\\
&\qquad+\frac{1}{2}\widetilde{\nabla}U^\intercal(\exp(V)^\intercal M\exp(V)-\exp(V)^\intercal M-M\exp(V)+M)\widetilde{\nabla}U.
\end{aligned}
\tag{9}
$$

On the other hand, it follows from the property of the DG (4) that

$$
\begin{aligned}
&U(y^1)-U(y^0)\\
&\quad=(y^{1\intercal}-y^{0\intercal})\overline{\nabla}U(y^1,y^0)\\
&\quad=y^{0\intercal}(\exp(V)^\intercal-I)\overline{\nabla}U+h\overline{\nabla}U^\intercal Q^\intercal\varphi(V)^\intercal\overline{\nabla}U\\
&\quad=y^{0\intercal}(\exp(V)^\intercal M-M)\widetilde{\nabla}U+\widetilde{\nabla}U^\intercal V^\intercal\varphi(V)^\intercal M\widetilde{\nabla}U\\
&\quad=y^{0\intercal}(\exp(V)^\intercal M-M)\widetilde{\nabla}U+\widetilde{\nabla}U^\intercal(\exp(V)^\intercal M-M)\widetilde{\nabla}U.
\end{aligned}
\tag{10}
$$

Combining (9), (10), and collecting terms by types "$y^{0\intercal}*y^0$," "$y^{0\intercal}*\widetilde{\nabla}U$," "$\widetilde{\nabla}U^\intercal*\widetilde{\nabla}U$" leads to

$$
\begin{aligned}
&H(y^1)-H(y^0)\\
&\quad=\frac{1}{2}y^{1\intercal}My^1-\frac{1}{2}y^{0\intercal}My^0+U(y^1)-U(y^0)\\
&\quad=\frac{1}{2}y^{0\intercal}(\exp(V)^\intercal M\exp(V)-M)y^0+y^{0\intercal}(\exp(V)^\intercal M\exp(V)-M)\widetilde{\nabla}U\\
&\qquad+\frac{1}{2}\widetilde{\nabla}U^\intercal(\exp(V)^\intercal M\exp(V)-M)\widetilde{\nabla}U+\frac{1}{2}\widetilde{\nabla}U^\intercal(\exp(V)^\intercal M-M\exp(V))\widetilde{\nabla}U\\
&\quad=\frac{1}{2}(y^0+\widetilde{\nabla}U)^\intercal B(y^0+\widetilde{\nabla}U)+\frac{1}{2}\widetilde{\nabla}U^\intercal C\widetilde{\nabla}U=0,
\end{aligned}
\tag{11}
$$

where $B=\exp(V)^\intercal M\exp(V)-M$ and $C=\exp(V)^\intercal M-M\exp(V)$. The last step is from the skew symmetry of the matrix $B$ (according to Lemma 2.2) and $C$.

If $M$ is singular, it is easy to find a series of symmetric and nonsingular matrices $\{M_\varepsilon\}$ which converge to $M$ when $\varepsilon\to 0$. Thus, according to the result stated above,

it still holds that

$$H_\varepsilon(y_\varepsilon^1) = H_\varepsilon(y^0) \tag{12}$$

for all $\varepsilon$, where $H_\varepsilon(y) = \frac{1}{2}y^\intercal M_\varepsilon y + U(y)$ is the first integral of the perturbed problem

$$\dot{y} = Q(M_\varepsilon y + \nabla U(y)), \quad y(t_0) = y^0,$$

and

$$y_\varepsilon^1 = \exp(V_\varepsilon)y^0 + h\varphi(V_\varepsilon)Q\overline{\nabla}U(y_\varepsilon^1, y^0), \quad V_\varepsilon = hQM_\varepsilon.$$

Therefore, when $\varepsilon \to 0$, $y_\varepsilon^1 \to y^1$ and (12) lead to

$$H(y^1) = H(y^0).$$

This completes the proof. ∎

Moreover, the scheme (7) can also model the decay of the Lyapunov function once $Q \le 0$ in (3). The next theorem shows this point.

THEOREM 2.4. *If $Q$ is negative semidefinite (not necessarily symmetric), then the scheme* (7) *preserves the Lyapunov function $H$ in* (3)*:*

$$H(y^1) \le H(y^0),$$

*where* $H(y) = \frac{1}{2}y^\intercal My + U(y)$.

*Proof.* If $M$ is nonsingular, the equation in (11)

$$H(y^1) - H(y^0) = \frac{1}{2}(y^0 + \widetilde{\nabla}U)^\intercal B(y^0 + \widetilde{\nabla}U)$$

still holds, since the derivation does not depend on the skew symmetry of $Q$. By Lemma 2.2, $B$ is negative semidefinite. Thus $H(y^1) \le H(y^0)$. In the case that $M$ is singular, this theorem can be easily proved by replacing the equalities

$$H_\varepsilon(y_\varepsilon^1) = H_\varepsilon(y^0), \quad H(y^1) = H(y^0)$$

in the proof of Theorem 2.3 with the inequalities

$$sH_\varepsilon(y_\varepsilon^1) \le H_\varepsilon(y^0), \quad H(y^1) \le H(y^0).$$

We here skip the details. ∎

In this paper, we choose the average vector field (AVF) as the DG in (7). The corresponding scheme for (3) now is

$$y^1 = \exp(V)y^0 + h\varphi(V)Q\int_0^1 \nabla U((1-\tau)y^0 + \tau y^1)d\tau, \tag{13}$$

where $V = hQM$ and $y^1 \approx y(t_0 + h)$. (13) is called an *exponential AVF integrator* and denoted by EAVF.

**3. Properties of EAVF.** In this section, we present two properties of EAVFs as follows.

THEOREM 3.1. *The EAVF integrator* (13) *is symmetric.*

*Proof.* Exchanging $y^0 \leftrightarrow y^1$ and replacing $h$ by $-h$ in (13), we obtain

$$y^0 = \exp(-V)y^1 - h\varphi(-V)Q\int_0^1 \nabla U((1-\tau)y^1 + \tau y^0)d\tau. \tag{14}$$

Rewrite (14) as

$$y^1 = \exp(V)y^0 + h\exp(V)\varphi(-V)Q\int_0^1 \nabla U((1-\tau)y^0 + \tau y^1)d\tau. \tag{15}$$

Since $\exp(V)\varphi(-V) = \varphi(V)$, (15) is the same as (13) exactly, which means that EAVF is symmetric. ∎

It should be noted that the scheme (13) is implicit in general, and thus iteration solutions are required. Next, we discuss the convergence of the fixed-point iteration for the EAVF integrator.

THEOREM 3.2. *Suppose that* $\|\varphi(V)\|_2 \le C$, $\nabla U(u)$ *satisfies the Lipschitz condition, i.e., there exists a constant* $L$ *such that*

$$\|\nabla U(v) - \nabla U(w)\|_2 \le L\|v - w\|_2.$$

*If*

$$0 < h \le \hat{h} < \frac{2}{CL\|Q\|_2}, \tag{16}$$

*then the iteration*

$$\Psi : z \mapsto \exp(V)y^n + h\varphi(V)Q\int_0^1 \nabla U((1-\tau)y^n + \tau z)d\tau$$

*for the EAVF integrator* (13) *is convergent.*

*Proof.* Since

$$\begin{aligned}
&\|\Psi(z_1) - \Psi(z_2)\|_2 \\
&\quad = \|h\varphi(V)Q\int_0^1 (\nabla U((1-\tau)y^n + \tau z_1) - \nabla U((1-\tau)y^n + \tau z_2))d\tau\|_2 \\
&\quad \le \frac{h}{2}CL\|Q\|_2\|z_1 - z_2\|_2 \le \frac{\hat{h}}{2}CL\|Q\|_2\|z_1 - z_2\|_2 = \rho\|z_1 - z_2\|_2,
\end{aligned}$$

where

$$\rho = \frac{\hat{h}}{2}CL\|Q\|_2 < 1,$$

the iteration $\Psi$ converges by (16) and the contraction mapping theorem. ∎

*Remark* 3.3. We note two special and important cases in practical applications. If $QM$ is skew symmetric or symmetric negative semidefinite, then the spectrum of $V$ lies in the left half-plane. Since $QM$ is unitarily diagonalizable and $|\varphi(z)| \le 1$ for any $z$ satisfying $real(z) \le 0$, we have $\|\varphi(V)\|_2 \le 1$.

In many cases, the matrix $M$ has an extremely large norm (e.g., $M$ incorporates high frequency components in oscillatory problems or $M$ is the differential matrix in semidiscrete PDEs), thus, Theorem 3.2 ensures the possibility of choosing a relatively large step size regardless of $M$.

In practice, the integral in (13) usually cannot be easily calculated. Therefore, we can evaluate it using the $s$-point Gauss–Legendre (GL$s$) formula $(b_i, c_i)_{i=1}^s$:

$$\int_0^1 \nabla U((1-\tau)y^0 + \tau y^1)d\tau \approx \sum_{i=1}^s b_i \nabla U((1-c_i)y^0 + c_i y^1)).$$

The corresponding scheme is denoted by EAVFGL$s$. Since the $s$-point GL quadrature formula is symmetric, EAVFGL$s$ is also symmetric. According to $\sum_{i=1}^s b_i c_i = 1/2$, the corresponding iteration for EAVFGL$s$ is convergent provided (16) holds.

## 4. Problems suitable for the EAVF.

**4.1. Highly oscillatory nonseparable Hamiltonian system.** Consider the Hamiltonian

$$H(p,q) = \frac{1}{2}p_1^\intercal M_1^{-1} p_1 + \frac{1}{2\varepsilon^2} q_1^\intercal A_1 q_1 + S(p,q),$$

where

$$p = \begin{pmatrix} p_0 \\ p_1 \end{pmatrix}, \quad q = \begin{pmatrix} q_0 \\ q_1 \end{pmatrix}$$

are both $d$-length vectors, $M_1, A_1$ are symmetric positive definite matrices, and $0 < \varepsilon \ll 1$. This Hamiltonian governs oscillatory mechanical systems in 2 or 3 space dimensions such as the stiff spring pendulum and the dynamics of the multiatomic molecule (see, e.g., [8, 9]). After an appropriate canonical transformation (see, e.g., [18]), this Hamiltonian becomes

$$H(p,q) = \frac{1}{2}\sum_{j=1}^{l}\left(p_{1,j}^2 + \frac{\lambda_j^2}{\varepsilon^2} q_{1,j}^2\right) + S(p,q), \tag{17}$$

where $p_1 = (p_{1,1}, \ldots, p_{1,l})^\intercal, q_1 = (q_{1,1}, \ldots, q_{1,l})^\intercal$. The corresponding equation is given by

$$\begin{cases} \dot{p_0} = -\nabla_{q_0} S(p,q), \\ \dot{p_1} = -\omega^{2\intercal} q_1 - \nabla_{q_1} S(p,q), \\ \dot{q_0} = p_0 + (\nabla_{p_0} S(p,q) - p_0), \\ \dot{q_1} = p_1 + \nabla_{p_1} S(p,q), \end{cases} \tag{18}$$

where $\omega = (\omega_1, \ldots, \omega_l)^\intercal, \omega_j = \lambda_j/\varepsilon$ for $j = 1, \ldots, l$. (18) is of the form (3):

$$y = \begin{pmatrix} p \\ q \end{pmatrix}, \quad Q = \begin{pmatrix} O & -I_{d\times d} \\ I_{d\times d} & O \end{pmatrix}, \quad M = \begin{pmatrix} I_{d\times d} & O \\ O & \Omega_{d\times d} \end{pmatrix},$$

and

$$U(p,q) = S(p,q) - \frac{1}{2}p_0^\intercal p_0, \quad \Omega = diag(0, \ldots, 0, \omega_1^2, \ldots, \omega_l^2).$$

Since $q_{11}, \ldots, q_{1l}$ and $p_{11}, \ldots, p_{1l}$ are fast variables, it is favorable to integrate the linear part of them exactly by the scheme (13). Note that

$$\varphi(V) = \begin{pmatrix} sinc(h\Omega^{\frac{1}{2}}) & h^{-1}g_2(h\Omega^{\frac{1}{2}}) \\ hg_1(h\Omega^{\frac{1}{2}}) & sinc(h\Omega^{\frac{1}{2}}) \end{pmatrix},$$

where $sinc(z) = \sin(z)/z, g_1(z) = (1-\cos(z))/z^2, g_2(z) = \cos(z) - 1$. Unfortunately, the block $h^{-1}g_2(h\Omega^{\frac{1}{2}})$ is not uniformly bounded. In the first experiment, the iteration still works well, perhaps due to the small Lipshitz constant of $\nabla S$.

**4.2. Second-order (damped) highly oscillatory system.** Consider

$$\ddot{q} - N\dot{q} + \Omega q = -\nabla U_1(q), \tag{19}$$

where $q$ is a $d$-length vector variable, $U_1 : \mathbb{R}^d \to \mathbb{R}$ is a differential function, $N$ is a symmetric negative semidefinite matrix, $\Omega$ is a symmetric positive semidefinite matrix, $\|\Omega\|$ or $\|N\| \gg 1$. Equation (19) stands for highly oscillatory problems such as the dissipative molecular dynamics, the (damped) Duffing and semidiscrete nonlinear wave equations. By introducing $p = \dot{q}$, we write (19) as a first-order system of ODEs:

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} O & I \\ -\Omega & N \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla U_1(q) \end{pmatrix}, \tag{20}$$

which falls into the class (3), where

$$y = \begin{pmatrix} q \\ p \end{pmatrix}, Q = \begin{pmatrix} O & I \\ -I & N \end{pmatrix}, M = \begin{pmatrix} \Omega & O \\ O & I \end{pmatrix}, U(y) = \begin{pmatrix} U_1(q) \\ O \end{pmatrix}.$$

Clearly, $Q \leq 0$ and (20) is a dissipative system with the Lyapunov function $H = \frac{1}{2}p^{\intercal}p + \frac{1}{2}q^{\intercal}\Omega q + U_1(q)$. In the particular case $N = 0$, (20) becomes a conservative Hamiltonian system. Let

$$A = QM = \begin{pmatrix} O & I \\ -\Omega & N \end{pmatrix}.$$

Applying the EAVF integrator (13) to (20) yields the scheme

$$\begin{cases} q^1 = \exp_{11} q^0 + \exp_{12} p^0 - h\varphi_{12} \displaystyle\int_0^1 \nabla U_1((1-\tau)q^0 + \tau q^1)d\tau, \\ p^1 = \exp_{21} q^0 + \exp_{22} p^0 - h\varphi_{22} \displaystyle\int_0^1 \nabla U_1((1-\tau)q^0 + \tau q^1)d\tau, \end{cases} \tag{21}$$

where $\exp(hA)$ and $\varphi(hA)$ are partitioned into

$$\begin{pmatrix} \exp_{11} & \exp_{12} \\ \exp_{21} & \exp_{22} \end{pmatrix} \text{ and } \begin{pmatrix} \varphi_{11} & \varphi_{12} \\ \varphi_{21} & \varphi_{22} \end{pmatrix},$$

respectively.

It should be noted that only the first equation in the scheme (21) needs to be solved by iteration. From the proof procedure of Theorem 3.2, one can find that the convergence of the fixed-point iteration for (21) is irrelevant to $\|A\|$ provided $\varphi_{12}$ is uniformly bounded.

THEOREM 4.1. *Assume that $\Omega$ commutes with $N$, $\|\nabla U_1(v) - \nabla U_1(w)\|_2 \leq L\|v - w\|_2$, then the iteration*

$$\Phi : z \mapsto \exp_{11} q^0 + \exp_{12} p^0 - h\varphi_{12} \int_0^1 \nabla U_1((1-\tau)q^0 + \tau z)d\tau$$

*for the scheme* (21) *is convergent provided*

$$0 < h \leq \hat{h} < \frac{2}{L^{\frac{1}{2}}}.$$

*Proof.* The crucial point here is to find a uniform upper bound of $\|\varphi_{12}\|$. Since $\Omega$ commutes with $N$, they can be simultaneously diagonalized:

$$\Omega = F^\intercal \Lambda F, \quad N = F^\intercal \Sigma F,$$

where $F$ is an orthogonal matrix, $\Lambda = diag(\lambda_1, \ldots, \lambda_d), \Sigma = diag(\sigma_1, \ldots, \sigma_d)$, and $\lambda_i \geq 0, \sigma_i \leq 0$ for $i = 1, 2, \ldots, d$. It now follows from

$$A = \begin{pmatrix} F^\intercal & O \\ O & F^\intercal \end{pmatrix} \begin{pmatrix} O & I \\ -\Lambda & \Sigma \end{pmatrix} \begin{pmatrix} F & O \\ O & F \end{pmatrix}$$

that

$$\exp(hA) = \begin{pmatrix} F^\intercal & O \\ O & F^\intercal \end{pmatrix} \exp\left\{ \begin{pmatrix} O & hI \\ -h\Lambda & h\Sigma \end{pmatrix} \right\} \begin{pmatrix} F & O \\ O & F \end{pmatrix}.$$

To show that $\exp_{12}$ and $\varphi_{12}$ depend on $h$, we denote them by $\exp_{12}^h$ and $\varphi_{12}^h$, respectively. After some calculations, we have

$$\exp_{12}^h = F^\intercal \frac{2\sinh(h(\Sigma^2 - 4\Lambda)^{\frac{1}{2}}/2)}{(\Sigma^2 - 4\Lambda)^{\frac{1}{2}}} \exp\left(\frac{h\Sigma}{2}\right) F.$$

Then we have

$$\begin{aligned} \| \exp_{12}^h \|_2 &= \left\| \frac{2\sinh(h(\Sigma^2 - 4\Lambda)^{\frac{1}{2}}/2)}{(\Sigma^2 - 4\Lambda)^{\frac{1}{2}}} \exp\left(\frac{h\Sigma}{2}\right) \right\|_2 \\ &= h \max_i \left| \frac{\sinh((h^2\sigma_i^2/4 - \lambda_i)^{\frac{1}{2}})}{(h^2\sigma_i^2/4 - \lambda_i)^{\frac{1}{2}}} \exp\left(\frac{h\sigma_i}{2}\right) \right|. \end{aligned} \tag{22}$$

In order to estimate $\| \exp_{12}^h \|_2$, the bound of the function

$$g(\lambda, \sigma) = \frac{\sinh((\sigma^2 - 4\lambda)^{\frac{1}{2}})}{(\sigma^2 - 4\lambda)^{\frac{1}{2}}} \exp(\sigma)$$

should be considered for $\sigma \leq 0, \lambda \geq 0$. If $\sigma^2 - 4\lambda < 0$, we set $(\sigma^2 - 4\lambda)^{\frac{1}{2}} = ia$, where $i$ is the imaginary unit and $a$ is a real number. Then we have

$$|g| = \left| \frac{\sin(a)}{a} \exp(\sigma) \right| \leq \left| \frac{\sin(a)}{a} \right| \leq 1.$$

If $\sigma^2 - 4\lambda \geq 0$, then $a = (\sigma^2 - 4\lambda)^{\frac{1}{2}} \leq -\sigma$,

$$|g| = \left| \frac{\sinh(a)}{a} \exp(\sigma) \right| \leq \left| \frac{\sinh(a)}{a} \exp(-a) \right| = \left| \frac{1 - \exp(-2a)}{2a} \right| \leq 1.$$

Thus

$$|g(\lambda, \sigma)| \leq 1 \quad \text{for } \sigma \leq 0, \lambda \geq 0. \tag{23}$$

It follows from (22) and (23) that

$$\| \exp_{12}^h \|_2 = h \max_i \left| g\left(\frac{h\sigma_i}{2}, \lambda_i\right) \right| \leq h. \tag{24}$$

Therefore, using $\varphi(hA) = \int_0^1 \exp((1-\xi)hA)d\xi$ and (24), we obtain

$$\|\varphi_{12}^h\|_2 = \left\| \int_0^1 \exp_{12}^{(1-\xi)h} d\xi \right\|_2 \le \int_0^1 \| \exp_{12}^{(1-\xi)h} \|_2 d\xi \le \int_0^1 (1-\xi)h d\xi = \frac{1}{2}h.$$

Since the rest of the proof is very similar to that of Theorem 3.2, we omit it here. ∎

It can be observed that in the particular case that $N = 0$, the scheme (21) reduces to the AAVF integrator in [31].

**4.3. Semidiscrete conservative and dissipative PDEs.** Many time-dependent PDEs are of the form

$$\partial_t y(x,t) = \mathcal{Q}\frac{\delta \mathcal{H}}{\delta y}, \tag{25}$$

where $y(\cdot,t) \in X$ for every $t \ge 0$, $X$ is a Hilbert space such as $\mathbf{L}^2(\Omega), \mathbf{L}^2(\Omega) \times \mathbf{L}^2(\Omega), \ldots$, $\Omega$ is a domain in $\mathbb{R}^d$, and $\mathcal{Q}$ is a linear operator on $X$. $\mathcal{H}[y] = \int_\Omega H(y, \partial_\alpha y)dx$ ($H$ is smooth, $x = (x_1, \ldots, x_d), dx = dx_1 \ldots dx_d$, and $\partial_\alpha y$ denotes the partial derivatives of $y$ with respect to spatial variables $x_i, 1 \le i \le d$). Under suitable boundary condition (BC), the variational derivative $\frac{\delta \mathcal{H}}{\delta y}$ is defined by

$$\left\langle \frac{\delta \mathcal{H}}{\delta y}, z \right\rangle = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \mathcal{H}[y + \varepsilon z]$$

for any smooth $z \in X$ satisfying the same BC, where $\langle \cdot, \cdot \rangle$ is the inner product of $X$. If $\mathcal{Q}$ is a skew or negative semidefinite operator with respect to $\langle \cdot, \cdot \rangle$, then (25) is conservative (e.g., the nonlinear wave, nonlinear Schrödinger (NLS), Korteweg–de Vries, and Maxwell equations) or dissipative (e.g., the Allen–Cahn (AC), Cahn–Hilliard, Ginzburg–Landau and heat equations), i.e., $\mathcal{H}[y]$ is constant or monotonically decreasing (see, e.g., [6, 13]). In general, after the spatial discretization, (25) becomes a conservative or dissipative system of ODEs in the form (3). Here we exemplify conservative ones by the NLS equation

$$iy_t + y_{xx} + V'(|y|^2)y = 0 \tag{26}$$

under the periodic BC $y(0,t) = y(L,t)$, where $y = p + iq$ is a complex-valued function, $p, q$ are both real, $i$ is the imaginary unit. Equation (26) is of the form (25)

$$\partial_t \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} p_{xx} + V'(p^2+q^2)p \\ q_{xx} + V'(p^2+q^2)q \end{pmatrix}, \tag{27}$$

where $X = \mathbf{L}^2([0,L]) \times \mathbf{L}^2([0,L]), \mathcal{H}[y] = \frac{1}{2}\int_0^L (V(p^2+q^2) - p_x^2 - q_x^2)dx$. Assume that the spatial domain is equally partitioned into $N$ intervals: $0 = x_0 < x_1 < \cdots < x_N = L$. Discretizing the spatial derivatives of (27) by the central difference arrives at

$$\begin{pmatrix} \dot{\tilde{p}} \\ \dot{\tilde{q}} \end{pmatrix} = \begin{pmatrix} O & -I \\ I & O \end{pmatrix} \begin{pmatrix} D\tilde{p} + V'(\tilde{p}^2+\tilde{q}^2)\tilde{p} \\ D\tilde{q} + V'(\tilde{p}^2+\tilde{q}^2)\tilde{q} \end{pmatrix}, \tag{28}$$

where

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

is an $N \times N$ symmetric differential matrix, $\tilde{p} = (p_0, \ldots, p_{N-1})^\intercal, \tilde{q} = (q_0, \ldots, q_{N-1})^\intercal$, $p_i(t) \approx p(x_i, t)$, and $q_i(t) \approx q(x_i, t)$ for $i = 0, \ldots, N-1$.

An example of dissipative PDEs is the AC equation:

$$y_t = dy_{xx} + y - y^3, \quad d \geq 0, \tag{29}$$

under the Neumann BC $y_x(0,t) = y_x(L,t)$. $X = \mathbf{L}^2([0,L]), \mathcal{Q} = -1, \mathcal{H}[y] = \int (\frac{1}{2} d y_x^2 - \frac{1}{2} y^2 + \frac{1}{4} y^4) dx$. The spatial grids are chosen in the same way as the NLS equation. Discretizing the spatial derivative by the central difference, we obtain

$$\dot{\tilde{y}} = d\hat{D}\tilde{y} + \tilde{y} - \tilde{y}^3, \tag{30}$$

where

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

is the $(N-1) \times (N-1)$ symmetric differential matrix, $\tilde{y} = (y_1, \ldots, y_{N-1})^\intercal, y_i(t) \approx y(x_i, t)$.

Both the semidiscrete NLS equation (28) and AC equation (30) are of the form (3). For the NLS and the AC equations, we have

$$Q = \begin{pmatrix} O & -I \\ I & O \end{pmatrix}, \quad M = \begin{pmatrix} D & O \\ O & D \end{pmatrix}, \quad U = \frac{1}{2} \sum_{i=0}^{N-1} V(p_i^2 + q_i^2),$$

and

$$Q = -I, \quad M = -d\hat{D}, \quad U = \sum_{i=1}^{N-1} \left( -\frac{1}{2} y_i^2 + \frac{1}{4} y_i^4 \right),$$

respectively. Therefore, the scheme (13) can be applied to solve them. Since the matrix $QM$ is skew or symmetric negative semidefinite in these two cases, according to Remark 3.3, the convergence of fixed-point iterations for them is independent of the differential matrix.

**5. Numerical experiments.** In this section, we compare the EAVF method (13) with the well-known implicit midpoint method which is denoted by MID:

$$y^1 = y^0 + hQ\nabla \widetilde{U}\left( \frac{y^0 + y^1}{2} \right), \tag{31}$$

and the traditional AVF method for (3) given by

$$y^1 = y^0 + hQ \int_0^1 \nabla \widetilde{U}((1-\tau)y^0 + \tau y^1) d\tau, \tag{32}$$

where $\widetilde{U}(y) = U(y) + \frac{1}{2} y^\intercal M y$. The authors in [28] showed that (32) preserves the first integral or the Lyapunov function $\widetilde{U}$. Our comparison also includes another

energy-preserving method of order four for (3):

$$\begin{cases} y^{\frac{1}{2}} = y^0 + hQ\displaystyle\int_0^1 \left(\frac{5}{4} - \frac{3}{2}\tau\right)\nabla\widetilde{U}(y_\tau)d\tau, \\ y^1 = y^0 + hQ\displaystyle\int_0^1 \nabla\widetilde{U}(y_\tau)d\tau, \end{cases} \tag{33}$$

where

$$y_\tau = (2\tau-1)(\tau-1)y^0 - 4\tau(\tau-1)y^{\frac{1}{2}} + (2\tau-1)\tau y^1.$$

This method can be written as a continuous Runge–Kutta (CRK) method. For details, readers are referred to [17].

Throughout the experiment, the "reference solution" is computed by high-order methods with a sufficiently small step size. We always start to calculate from $t_0 = 0$. $y^n \approx y(t_n)$ is obtained by the time-stepping way $y^0 \to y^1 \to \cdots \to y^n \to \cdots$ for $n = 1, 2, \ldots$ and $t_n = nh$. The error tolerance for iteration solutions of the four methods is set as $10^{-14}$. The maximum global error (GE) over the total time interval is defined by

$$GE = \max_{n\geq 0} \|y^n - y(t_n)\|_\infty.$$

The maximum global error of $H$ ($EH$) on the interval is

$$EH = \max_{n\geq 0} |H^n - H(y(t_n))|.$$

In our numerical experiments, the computational cost of each method is measured by the number of function evaluations (FE).

PROBLEM 5.1. *The motion of a triatomic molecule can be modeled by a Hamiltonian system with the Hamiltonian of the form* (17) *(see, e.g.,* [8]*):*

$$H(p,q) = S(p,q) + \frac{1}{2}(p_{1,1}^2 + p_{1,2}^2 + p_{1,3}^2) + \frac{\omega^2}{2}(q_{1,1}^2 + q_{1,2}^2 + q_{1,3}^2), \tag{34}$$

*where*

$$S(p,q) = \frac{1}{2}p_0^2 + \frac{1}{4}(q_0 - q_{1,3})^2 - \frac{1}{4}\frac{2q_{1,2} + q_{1,2}^2}{(1+q_{1,2})^2}(p_0 - p_{1,3})^2 - \frac{1}{4}\frac{2q_{1,1} + q_{1,1}^2}{(1+q_{1,1})^2}(p_0 + p_{1,3})^2.$$

*The initial values are given by*

$$\begin{cases} p_0(0) = p_{1,1}(0) = p_{1,2}(0) = p_{1,3}(0) = 1, \\ q_0(0) = 0.4, q_{1,1}(0) = q_{1,2}(0) = \dfrac{1}{\omega}, q_{1,3} = \dfrac{1}{2^{\frac{1}{2}}\omega}. \end{cases}$$

*Setting* $h = 1/2^i, i = 6, \ldots, 10, \omega = 50$, *and* $h = 1/100 \times 1/2^i, i = 0, \ldots, 4, \omega = 100$, *we integrate the problem* (18) *with the Hamiltonian* (34) *over the interval* $[0, 50]$. *Since the nonlinear term* $\nabla S(p,q)$ *is complicated to integrate, we evaluate the integrals in EAVF, AVF, and CRK by the* 3*-point GL quadrature formula* $(b_i, c_i)_{i=1}^3$*:*

$$b_1 = \frac{5}{18}, b_2 = \frac{4}{9}, b_3 = \frac{5}{18}; \quad c_1 = \frac{1}{2} - \frac{15^{\frac{1}{2}}}{10}, c_2 = \frac{1}{2}, c_3 = \frac{1}{2} + \frac{15^{\frac{1}{2}}}{10}.$$

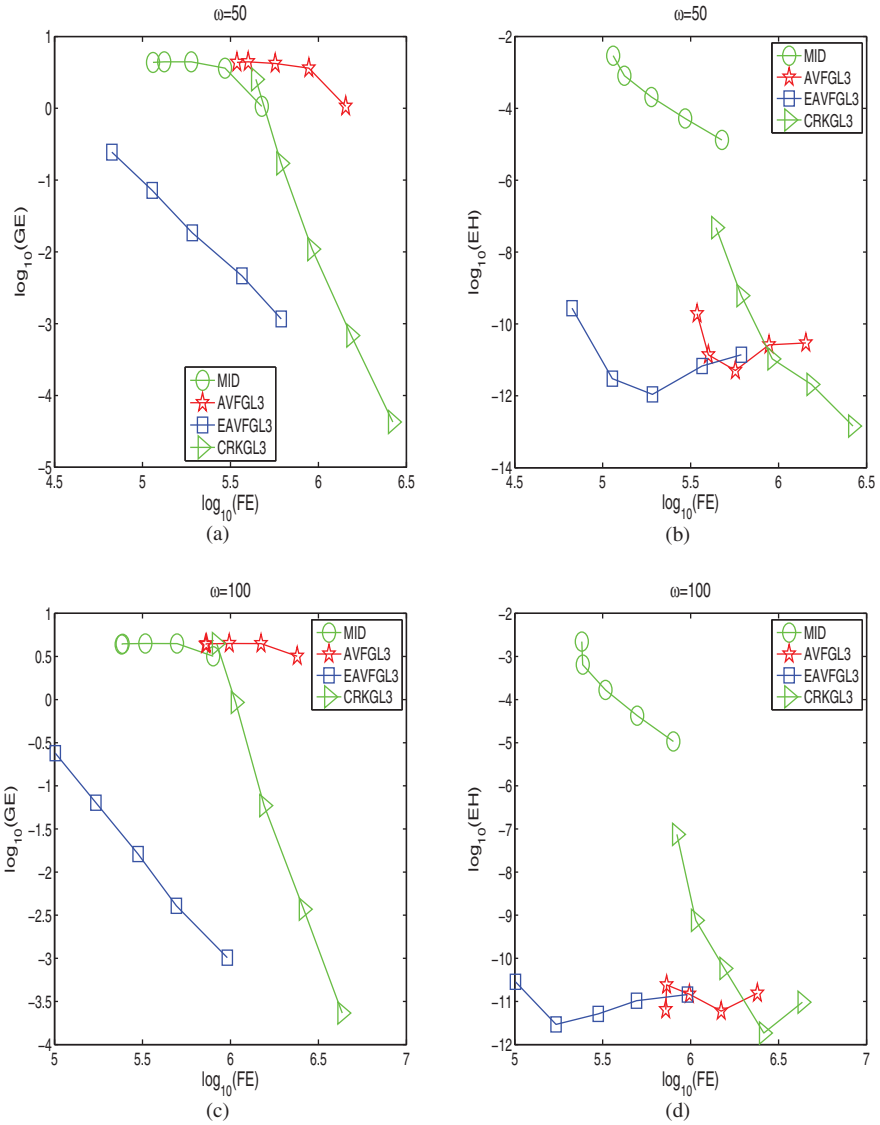


FIG. 1. *Efficiency curves.*

*Corresponding schemes are denoted by EAVFGL3, AVFGL3, and CRKGL3, respectively. Numerical results are presented in Figure* 1.

*Figures* 1(a) *and* 1(c) *show that MID and AVFGL3 lost basic accuracy. It can be observed from* 1(b) *and* 1(d) *that AVFGL3, EAVFGL3, CRKGL3 are much more efficient in preserving energy than MID. In the aspects of both energy preservation and algebraic accuracy, EAVF is the most efficient among the four methods.*

PROBLEM 5.2. *The equation*

$$\begin{aligned} \dot{x}_1 &= -\zeta x_1 - \lambda x_2 + x_1 x_2, \\ \dot{x}_2 &= \lambda x_1 - \zeta x_2 + \frac{1}{2}(x_1^2 - x_2^2), \end{aligned} \tag{35}$$

*is an averaged system in wind-induced oscillation, where* $\zeta \geq 0$ *is a damping factor and* $\lambda$ *is a detuning parameter (see, e.g.,* [16]*). For convenience, setting* $\zeta = rcos(\theta), \lambda = rsin(\theta), r \geq 0, 0 \leq \theta \leq \pi/2$*, (see* [29]*) we write* (35) *as*

(36)
$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} -\cos(\theta) & -\sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{pmatrix} \begin{pmatrix} rx_1 - \frac{1}{2}\sin(\theta)(x_2^2 - x_1^2) - \cos(\theta)x_1x_2 \\ rx_2 - \sin(\theta)x_1x_2 + \frac{1}{2}\cos(\theta)(x_2^2 - x_1^2) \end{pmatrix},$$

*which is of the form* (3)*, where*

(37)
$$Q = \begin{pmatrix} -\cos(\theta) & -\sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{pmatrix},$$
$$M = \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix}, \quad U = -\frac{1}{2}\sin(\theta)\left(x_1x_2^2 - \frac{1}{3}x_1^3\right) + \frac{1}{2}\cos(\theta)\left(\frac{1}{3}x_2^3 - x_1^2x_2\right).$$

*Its Lyapunov function (dissipative case, when* $\theta < \pi/2$*) or the first integral (conservative case, when* $\theta = \pi/2$*) is*

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

*The matrix exponential of the EAVF scheme* (13) *for* (36) *is calculated by*

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

*where* $c = \cos(\theta), s = \sin(\theta)$*, and* $\varphi(V)$ *can be obtained by* $(\exp(V) - I)V^{-1}$*. Given the initial values*

$$x_1(0) = 0, x_2(0) = 1,$$

*we first integrate the conservative system* (36) *with the parameters* $\theta = \pi/2, r = 20$ *and step sizes* $h = 1/20 \times 1/2^i, i = -1, \ldots, 4$*, over the interval* $[0, 200]$*. Setting* $\theta = \pi/2 - 10^{-4}, r = 20$*, we then integrate the dissipative* (36) *with the step sizes* $h = 1/20 \times 1/2^i, i = -1, \ldots, 4$*, over the interval* $[0, 100]$*. Numerical errors are presented in Figures* 2, 3*. It is noted that the integrands appearing in AVF, EAVF are polynomials of degree two and the integrands in CRK are polynomials of degree five. We evaluate the integrals in AVF, EAVF by the* 2*-point GL quadrature*

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

*and the integrals appearing in CRK by the* 3*-point GL quadrature. Then there is no quadrature error.*

*The efficiency curves of AVF and MID consist of only five points in Figures* 2(a), 2(b), 3(a) *(two points overlap in Figures* 2(a), 3(a)*), since the fixed-point iterations of MID and AVF are not convergent when* $h = 1/10$*. Note that* $QM$ *is skew symmetric or negative semidefinite, the convergence of iterations for the EAVF method is independent of* $r$ *by Theorem* 3.2 *and Remark* 3.3*. Thus larger step sizes are allowed for EAVF. The experiment shows that the iterations of EAVF uniformly work for* $h = 1/20 \times 1/2^i, i = -1, \ldots, 4$*. Moreover, it can be observed from Figure* 3(b) *that MID cannot strictly preserve the decay of the Lyapunov function.*

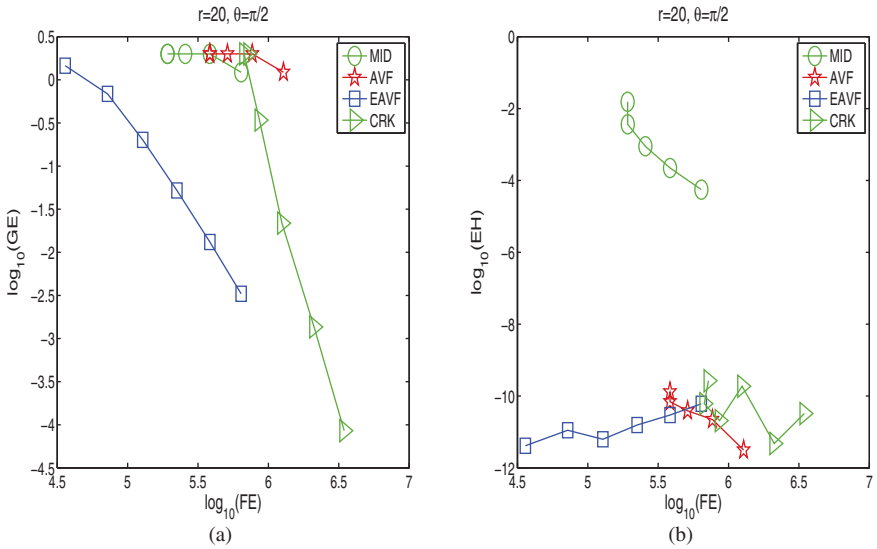


FIG. 2. *Efficiency curves.*

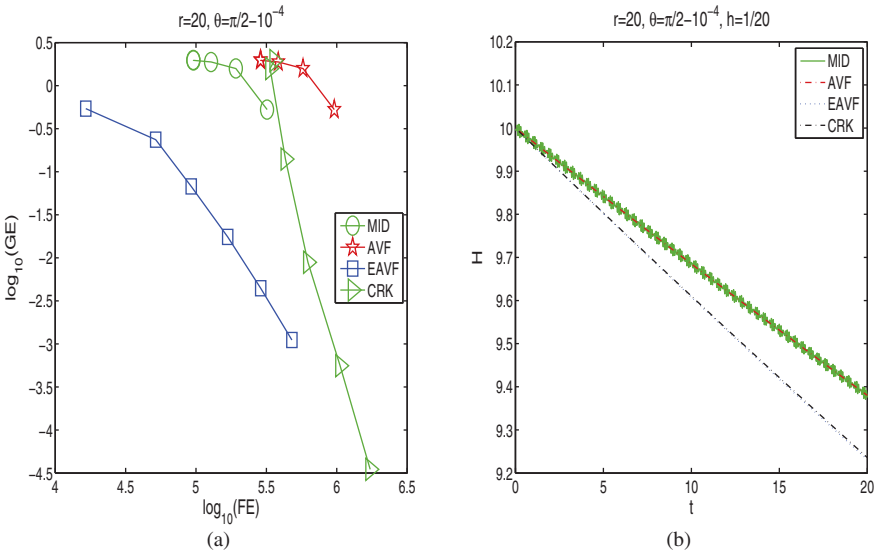


FIG. 3. (a) *Efficiency curves.* (b) *The Lyapunov function against time* $t$.

PROBLEM 5.3. *The PDE*

$$\frac{\partial^2 u}{\partial t^2} = \beta \frac{\partial^3 u}{\partial t \partial x^2} + \frac{\partial^2 u}{\partial x^2}\left(1 + \varepsilon \left(\frac{\partial u}{\partial x}\right)^p\right) - \gamma \frac{\partial u}{\partial t} - m^2 u, \tag{38}$$

*where* $\varepsilon > 0, \beta, \gamma \geq 0$, *is a continuous generalization of an* $\alpha$*-FPU (Fermi–Pasta–Ulam) system (see, e.g.,* [27]*). Taking* $\partial_t u = v$ *and the homogeneous Dirichlet BC*

$u(0,t) = u(L,t) = 0$, (38) *is of the type* (25), *where* $X = \mathbf{L}^2([0,L]) \times \mathbf{L}^2([0,L])$ *and*

$$y = \begin{pmatrix} u \\ v \end{pmatrix}, \quad \mathcal{Q} = \begin{pmatrix} 0 & 1 \\ -1 & \beta\partial_x^2 - \gamma \end{pmatrix},$$
$$\mathcal{H}[y] = \int_0^L \left( \frac{1}{2}u_x^2 + \frac{m^2}{2}u^2 + \frac{v^2}{2} + \frac{\varepsilon u_x^{p+2}}{(p+2)(p+1)} \right) dx.$$

*It is easy to verify that* $\mathcal{Q}$ *is a negative semidefinite operator, and thus* (38) *is dissipative. The spatial discretization yields a dissipative system of ODEs:*

$$\ddot{u}_j(t) - c^2(u_{j-1} - 2u_j + u_{j+1}) + m^2 u_j - \beta^{'}(\dot{u}_{j-1} - 2\dot{u}_j + \dot{u}_{j+1}) + \gamma\dot{u}_j(t) = \varepsilon^{'}(V^{'}(u_{j+1} - u_j) - V^{'}(u_j - u_{j-1})),$$

*where* $c = 1/\Delta x, \beta^{'} = c^2\beta, \varepsilon^{'} = c^{p+2}\varepsilon, V(u) = u^{p+2}/[(p+2)(p+1)], u_j(t) \approx u(x_j,t)$, $x_j = j/\Delta x$ *for* $j = 1, \ldots, N-1$, *and* $u_0(t) = u_N(t) = 0$. *Note that the nonlinear term* $u_{xx}u_x^p$ *is approximated by*

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

*We now write it in the compact form* (19)

$$\ddot{q} - N\dot{q} + \Omega q = -\nabla U_1(q),$$

$$q = (u_1, \ldots, u_{N-1})^{\intercal}, N = \beta^{'}D - \gamma I, \Omega = -c^2 D + m^2 I, U_1(q) = \varepsilon^{'}\sum_{j=0}^{N-1} V(u_{j+1} - u_j),$$

*and*

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

*In this experiment, we set* $p = 1, m = 0, c = 1, \varepsilon = \frac{3}{4}$, *and* $\gamma = 0.005$. *Consider the initial conditions in* [27]

$$\phi_j(t) = B\ln\left\{\left(\frac{1+\exp[2(\kappa(j-97)+t\sinh(\kappa))]}{1+\exp[2(\kappa(j-96)+t\sinh(\kappa))]}\right)\left(\frac{1+\exp[2(\kappa(j-32)+t\sinh(\kappa))]}{1+\exp[2(\kappa(j-33)+t\sinh(\kappa))]}\right)\right\}$$

*with* $B = 5, \kappa = 0.1$, *that is,*

$$\begin{cases} u_j(0) = \phi_j(0), \\ v_j(0) = \dot{\phi}_j(0) \end{cases}$$

*for* $j = 1, \ldots, N-1$. *Let* $N = 128, \beta = 0, 2$. *We compute the numerical solution by MID, AVF, and EAVF with the step sizes* $h = 1/2^i, i = 1, \ldots, 5$, *over the time*

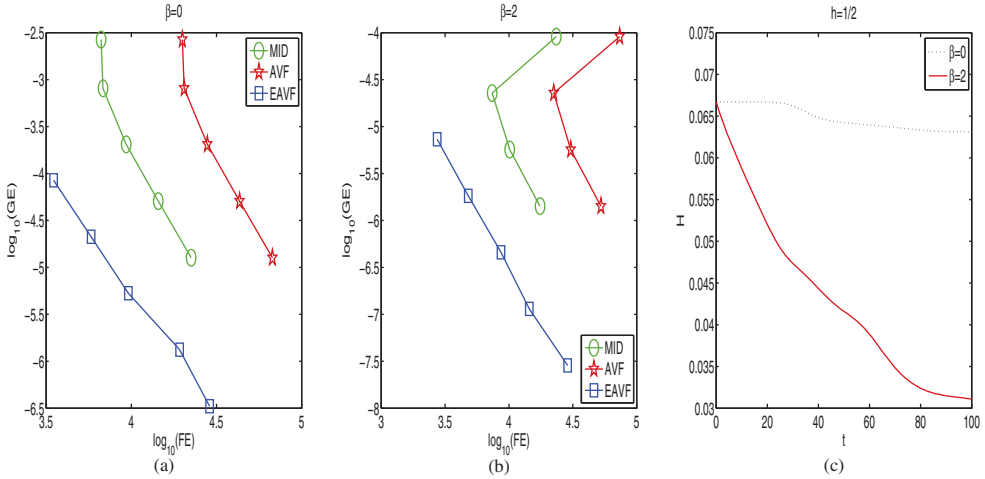


FIG. 4. (a) (b) *Efficiency curves.* (c) *The decay of the Lyapunov function obtained by EAVF.*

*interval* $[0, 100]$. *Similarly to EAVF* (21), *the nonlinear systems resulting from MID* (31) *and AVF* (32) *can be reduced to*

$$q^1 = q^0 + hp^0 + \frac{h}{2}N(q^1 - q^0) - \frac{h^2}{4}\Omega(q^1 + q^0) - \frac{h^2}{2}\nabla U_1\left(\frac{q^0 + q^1}{2}\right)$$

*and*

$$q^1 = q^0 + hp^0 + \frac{h}{2}N(q^1 - q^0) - \frac{h^2}{4}\Omega(q^1 + q^0) - \frac{h^2}{2}\int_0^1 \nabla U_1((1-\tau)q^0 + \tau q^1)d\tau,$$

*respectively. Both the velocity* $p^1$ *of MID and AVF can be recovered by*

$$\frac{q^1 - q^0}{h} = \frac{p^1 + p^0}{2}.$$

*The integrals in AVF and EAVF are exactly evaluated by the 2-point GL quadrature. Since* $\exp(hA), \varphi(hA)$ *in* (21) *have no explicit expressions, they are calculated by the MATLAB package in* [2]. *The basic idea is evaluating* $\exp(hA), \varphi(hA)$ *by their Padé approximations. Numerical results are plotted in Figure* 4. *Alternatively, there are other popular algorithms such as the contour integral method and the Krylov subspace method for matrix exponentials and* $\varphi$*-functions. Readers are referred to* [23] *for a summary of algorithms and well-established mathematical software.*

*According to Theorem* 4.1, *the convergence of iterations in the EAVF scheme is independent of* $\Omega$ *and* $N$. *Iterations of MID and AVF are not convergent when* $\beta = 2, h = 1/2$. *Thus the efficiency curves of MID and AVF in Figure* 4(b) *consist of only* 4 *points. From Figure* 4(c), *it can be observed that the EAVF method can preserve dissipation even using the relatively large step size* $h = 1/2$.

**6. Conclusions.** Exponential integrators can be traced back to the original paper by Hersch [20]. The term "exponential integrators" was coined in the seminal paper by Hochbruck, Lubich, and Selhofer [22]. It turns out that exponential integrators have constituted an important class of schemes for the numerical simulation of differential equations. In this paper, combining the ideas of the exponential integra-

tor with the average vector field, we derived and analyzed a new exponential scheme EAVF preserving the first integral or the Lyapunov function for the conservative or dissipative system (3), which includes numerous important mathematical models in applications. The symmetry of EAVF ensures the prominent long-term numerical behavior. Due to the implicity of EAVF requiring iteration solutions, we analyzed the convergence of the fixed-point iteration and showed that the convergence is free from the influence of a wide range of coefficient matrices $M$. In the dynamics of the triatomic molecule, the wind-induced oscillation, and the damped FPU problem, we compared the new EAVF method with the MID, AVF, and CRK methods. The three problems are modeled by the system (3) having a dominant linear term and small nonlinear term. In the aspects of algebraic accuracy as well as preserving energy and dissipation, EAVF is very efficient among the four methods. In general, energy-preserving and energy-decaying methods are implicit, and then iteration solutions are required. With a relatively large step size, the iterations of EAVF are convergent, whereas AVF and MID do not work in experiments. Therefore, EAVF is expected to be a promising method solving the system (3) with $\|QM\| \gg \|QHess(U)\|$.

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