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NUMERICAL ANALYSIS OF AN ENERGY-CONSERVATION SCHEME FOR TWO-DIMENSIONAL HAMILTONIAN WAVE EQUATIONS WITH NEUMANN BOUNDARY CONDITIONS

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Abstract. In this paper, an energy-conservation scheme is derived and analysed for solving Hamiltonian wave equations subject to Neumann boundary conditions in two dimensions. The energy-conservation scheme is based on the blend of spatial discretisation by a fourth-order finite difference method and time integration by the Average Vector Field (AVF) approach. The spatial discretisation via the fourth-order finite difference leads to a particular Hamiltonian system of second-order ordinary differential equations. The conservative law of the discrete energy is established, and the stability and convergence of the semi-discrete scheme are analysed. For the time discretisation, the corresponding AVF formula is derived and applied to the particular Hamlitonian ODEs to yield an efficient energy-conservation scheme. The numerical simulation is implemented for various cases including a linear wave equation and two nonlinear sine-Gordon equations. The numerical results demonstrate the spatial accuracy and the remarkable energy-conservation behaviour of the proposed energy-conservation scheme in this paper.

Key words. Two-dimensional Hamiltonian wave equation, finite difference method, Neumann boundary conditions, energy-conservation algorithm, average vector field formula.

1. Introduction

The theme of this paper is the numerical analysis of an energy-conservation scheme for the following Hamiltonian wave equation in two-dimensional space:

$$(1)\qquad \begin{cases} u_{tt}-a^2(u_{xx}+u_{yy})=f(u), & (x,y,t)\in\mathbf{\Omega}\times(t_0,T],\\ u(x,y,t_0)=\varphi(x,y),\ u_t(x,y,t_0)=\phi(x,y), & (x,y)\in\bar{\mathbf{\Omega}}, \end{cases}$$

where the function $f(u)$ is the negative derivative of a potential energy $V(u)$, and $\mathbf{\Omega}=(x_l,x_r)\times(y_d,y_u)$. The initial functions φ and ϕ are wave modes or kinks and their velocity, respectively (see, e.g. [22, 23, 38]). Here, we suppose that the system (1) is supplemented with the homogenous *Neumann boundary conditions:*

$$(2)\qquad \frac{\partial u}{\partial x}\Big|_{x=x_r,x_l}=0,\quad y_d\le y\le y_u,\quad \frac{\partial u}{\partial y}\Big|_{y=y_d,y_u}=0,\quad x_l\le x\le x_r,\quad \forall t\in[t_0,T].$$

It is noted that the conservation of the energy is an essential property of the Hamiltonian system (1)-(2), which can be expressed as follows:

$$(3)\qquad E(t)\equiv\frac{1}{2}\int_{\mathbf{\Omega}}\Big[u_t^2+a^2\big(u_x^2+u_y^2\big)+2V(u)\Big]\mathrm{d}x\mathrm{d}y=E(t_0).$$

Therefore, it is very important to design numerical schemes that can precisely preserve a discrete energy. This class of schemes is called conservative schemes. They often yield physically correct results and numerical stability [8].

In the literature, a considerable number of numerical schemes has been presented for solving the two-dimensional Hamiltonian wave equations (1). For example,

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Bratsos [5] applied the method of lines to solve system (1). In [13], the authors constructed a high-order compact alternating direction implicit scheme. Based on the blend of spatial discretisation by different finite difference methods and time integration by predictor-corrector schemes, the authors (see, e.g. [9, 12, 17]) investigated nonlinear Hamiltonian wave equations numerically. Dehghan et al. (see, e.g. [14, 15, 34, 35]) proposed the meshless local Petrov-Galerkin (MLPG) method, the meshless local radial point interpolation (LRPI) method, the dual reciprocity boundary element (DRBE) method and the meshless local boundary integral equation (LBIE) method for solving the two-dimensional sine-Gordon equations. In [29, 30, 31], Liu et al. first formulated the system (1) as an abstract second-order ODEs in a suitable infinite-dimensional function space and then proposed and analysed a class of arbitrarily high-order time-stepping methods for solving Hamiltonian system (1). Mei et al. [33] presented an extension of the finite-energy condition for Runge–Kutta–Nyström-type integrators solving nonlinear wave equations. The other numerical approaches also were investigated, such as the finite element method (see, e.g. [1, 2]), the perturbation method [24] and the spectral method (see, e.g. [3, 28]). On the other hand, splitting methods (see, e.g. [9, 11, 16, 17, 37]) have been developed to investigate the numerical solutions of the evolutional PDEs in multi-dimensional case. Sheng et al. [38] provided highly efficient splitting cosine schemes for the two-dimensional sine-Gordon equations by using a linearly implicit sequential splitting or Strangs splitting. In a recent study of Hamiltonian wave equations, using the finite difference method and the average vector field (AVF) method, the authors consider a class of energy-conservation methods for one-dimensional Hamiltonian wave equations (see [26]). However, there are very few studies to pay attention to designing and analysing high-order energy-conserving schemes for the two-dimensional Hamiltonian wave equations subject to Neumann boundary conditions. Hence, in this work, we devote to constructing and analysing a novel and efficient energy-conservation scheme for the Hamiltonian wave equations with Neumann boundary conditions (1)-(2) in two dimensions. According to the homogenous Neumann boundary conditions and the structure of equation (1), we derive and analysis a kind of fourth-order finite difference operators to discrete the spatial derivatives of the system (1)-(2). In such a way, the conserved PDEs can be converted into a particular Hamiltonian system of ODEs expressed in the form $Aw''(t) + Bw(t) = \tilde{f}\big(w(t)\big)$, and the Hamiltonian of the obtained ODEs can be thought of as the approximate energy of the original continuous system. This motivates us to consider the AVF approach to the discretisation of the derived Hamiltonian ODEs' system in time. Therefore, incorporating the fourth-order finite difference discretisation in space with the AVF time integrator yields a novel and efficient energy-conservation numerical scheme for the two-dimensional Hamiltonian wave equations (1)-(2).

The paper is organised as follows. In Section 2, a particluar Hamiltonian ODEs' system is obtained by applying the fourth-order finite difference operators to discrete the spatial derivatives of the nonlinear system (1)-(2). Then the conservation law, the stability and the convergence of the semi-discrete scheme are rigorously analysed. Section 3 is devoted to describing in detail the idea of the AVF formula for the derived Hamiltonian system of ODEs. In Section 4, numerical experiments on a linear Klein-Gordon equation and two sine-Gordon equations are implemented and the numerical results show the convergence order of the spatial discretisation and the excellent conservative property of the proposed numerical scheme. Section 5 is concerned with conclusions.

2. Energy-conservation spatial discretisation via a fourth-order finite difference method

In this section, we first present an energy-conservation finite difference scheme for the two-dimensional Hamiltonian wave equations (1)-(2), which is of order four for all the spatial grid points. Then the energy conservation law, the stability and the convergence of the semi-discrete scheme are rigorously analysed.

2.1. Notations and auxiliary lemmas. Suppose M_1 and M_2 are two positive integers. let $h_1 = \frac{x_r - x_l}{M_1}$ and $h_2 = \frac{y_u - y_d}{M_2}$ be the stepsizes of spatial direction and discretise the region $[x_l, x_r] \times [y_d, y_u]$ with the spatial grid $\mathbf{\Omega}_h = \big\{(x_i, y_j) \mid x_i = x_l + ih_1, y_j = y_d + jh_2,\ 0 \le i \le M_1, 0 \le j \le M_2\big\}$. For any grid function $u = \{u_{ij} \mid (x_i, y_j) \in \mathbf{\Omega}_h\}, v = \{v_{ij} \mid (x_i, y_j) \in \mathbf{\Omega}_h\}$, we use the following notations

$$\delta_x u_{i+\frac{1}{2},j} = \frac{u_{i+1,j} - u_{ij}}{h_1}, \quad \delta_x^2 u_{ij} = \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h_1^2},$$
$$\Delta_x u_{ij} = \frac{u_{i+1,j} - u_{i-1,j}}{2h_1}, \quad \Delta_x^2 u_{ij} = \frac{u_{i+2,j} - 2u_{ij} + u_{i-2,j}}{4h_1^2},$$

and two finite difference operators

$$-\mathcal{A}_x u_{ij} = \begin{cases} \dfrac{7}{3h_1}\delta_x u_{\frac{1}{2},j} - \dfrac{1}{6}\delta_x^2 u_{1,j}, & i = 0, \\ -\dfrac{1}{6h_1}\delta_x u_{\frac{1}{2},j} + \dfrac{7}{6}\delta_x^2 u_{1,j} - \dfrac{1}{12}\delta_x^2 u_{2,j}, & i = 1, \\ \dfrac{4}{3}\delta_x^2 u_{ij} - \dfrac{1}{3}\Delta_x^2 u_{ij}, & 2 \le i \le M_1 - 2, \\ \dfrac{1}{6h_1}\delta_x u_{M_1-\frac{1}{2},j} + \dfrac{7}{6}\delta_x^2 u_{M_1-1,j} - \dfrac{1}{12}\delta_x^2 u_{M_1-2,j}, & i = M_1 - 1, \\ -\dfrac{7}{3h_1}\delta_x u_{M_1-\frac{1}{2},j} - \dfrac{1}{6}\delta_x^2 u_{M_1-1,j}, & i = M_1, \end{cases} \tag{4}$$

and

$$-\mathcal{A}_y u_{ij} = \begin{cases} \dfrac{7}{3h_2}\delta_y u_{i,\frac{1}{2}} - \dfrac{1}{6}\delta_y^2 u_{i,1}, & j = 0, \\ -\dfrac{1}{6h_2}\delta_y u_{i,\frac{1}{2}} + \dfrac{7}{6}\delta_y^2 u_{i,1} - \dfrac{1}{12}\delta_y^2 u_{i,2}, & j = 1, \\ \dfrac{4}{3}\delta_y^2 u_{ij} - \dfrac{1}{3}\Delta_y^2 u_{ij}, & 2 \le j \le M_2 - 2, \\ \dfrac{1}{6h_2}\delta_y u_{i,M_2-\frac{1}{2}} + \dfrac{7}{6}\delta_y^2 u_{i,M_2-1} - \dfrac{1}{12}\delta_y^2 u_{i,M_2-2}, & j = M_2 - 1, \\ -\dfrac{7}{3h_2}\delta_y u_{i,M_2-\frac{1}{2}} - \dfrac{1}{6}\delta_y^2 u_{i,M_2-1}, & j = M_2. \end{cases} \tag{5}$$

Furthermore, by defining the inner product

$$\begin{aligned} \big(u, v\big) =& h_1 h_2 \Big[\frac{1}{4}\big(u_{0,0}v_{0,0} + u_{M_1,0}v_{M_1,0} + u_{0,M_2}v_{0,M_2} + u_{M_1,M_2}v_{M_1,M_2}\big) \\ &+ \frac{1}{2}\sum_{i=1}^{M_1-1}\big(u_{i,0}v_{i,0} + u_{i,M_2}v_{i,M_2}\big) \\ &+ \frac{1}{2}\sum_{j=1}^{M_2-1}\big(u_{0,j}v_{0,j} + u_{M_1,j}v_{M_1,j}\big) + \sum_{i=1}^{M_1-1}\sum_{j=1}^{M_2-1} u_{ij}v_{ij}\Big], \end{aligned} \tag{6}$$

the notations of the discrete l_2-norm $\|u\| = \sqrt{(u,u)}$ and other discrete norms

$$\|\delta_x u\|^2 = h_1 h_2 \sum_{i=0}^{M_1-1}\Big[\frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},0}\big)^2 + \sum_{j=1}^{M_2-1}\big(\delta_x u_{i+\frac{1}{2},j}\big)^2 + \frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},M_2}\big)^2\Big],$$

$$\|\Delta_x u\|^2 = h_1 h_2 \sum_{i=1}^{M_1-1}\Big[\frac{1}{2}\big(\Delta_x u_{i,0}\big)^2 + \sum_{j=1}^{M_2-1}\big(\Delta_x u_{i,j}\big)^2 + \frac{1}{2}\big(\Delta_x u_{i,M_2}\big)^2\Big],$$

can be yielded. Likewise, the notations $\delta_y u_{i,j+\frac{1}{2}},\ \delta_y^2 u_{ij},\ \Delta_y u_{ij},\ \Delta_y^2 u_{ij},\ \|\delta_y u\|^2$ and $\|\Delta_y u\|^2$ can be defined as well.

Lemma 2.1. *For any grid function $u = \{u_{ij} \mid (x_i, y_j) \in \mathbf{\Omega}_h\}$, we define the norm $\|\cdot\|_*$ by*

$$\|u\|_*^2 = \frac{4}{3}\big(\|\delta_x u\|^2 + \|\delta_y u\|^2\big) - \frac{1}{3}\big(\|\Delta_x u\|^2 + \|\Delta_y u\|^2\big), \tag{7}$$

and then, the following inequality holds

$$|u|_1^2 \le \|u\|_*^2, \tag{8}$$

where the H_1 semi-norm is given by $|u|_1^2 = \|\delta_x u\|^2 + \|\delta_y u\|^2$.

Proof. It follows from the definition of the operators $\Delta_x u_{ij}, \Delta_y u_{ij}$ and the norms $\|\Delta_x u\|, \|\Delta_x u\|$ that

$$\begin{aligned}\|\Delta_x u\|^2 =&\frac{h_1 h_2}{4}\sum_{i=1}^{M_1-1}\Big[\frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},0} + \delta_x u_{i-\frac{1}{2},0}\big)^2 + \sum_{j=1}^{M_2-1}\big(\delta_x u_{i+\frac{1}{2},j} + \delta_x u_{i-\frac{1}{2},j}\big)^2\\ &+ \frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},M_2} + \delta_x u_{i-\frac{1}{2},M_2}\big)^2\Big]\\ \le&\frac{h_1 h_2}{2}\sum_{i=0}^{M_1-1}\Big[\frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},0}\big)^2 + \sum_{j=1}^{M_2-1}\big(\delta_x u_{i+\frac{1}{2},j}\big)^2 + \frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},M_2}\big)^2\Big]\\ =&\|\delta_x u\|^2,\end{aligned}$$

and

$$\begin{aligned}\|\Delta_y u\|^2 =&\frac{h_1 h_2}{4}\sum_{j=1}^{M_2-1}\Big[\frac{1}{2}\big(\delta_y u_{0,j+\frac{1}{2}} + \delta_y u_{0,j-\frac{1}{2}}\big)^2 + \sum_{i=1}^{M_1-1}\big(\delta_y u_{i,j+\frac{1}{2}} + \delta_y u_{i,j-\frac{1}{2}}\big)^2\\ &+ \frac{1}{2}\big(\delta_y u_{M_1,j+\frac{1}{2}} + \delta_y u_{M_1,j-\frac{1}{2}}\big)^2\Big]\\ \le&\frac{h_1 h_2}{2}\sum_{j=0}^{M_2-1}\Big[\frac{1}{2}\big(\delta_y u_{0,j+\frac{1}{2}}\big)^2 + \sum_{i=1}^{M_1-1}\big(\delta_y u_{i,j+\frac{1}{2}}\big)^2 + \frac{1}{2}\big(\delta_y u_{M_1,j+\frac{1}{2}}\big)^2\Big]\\ =&\|\delta_y u\|^2.\end{aligned}$$

We then obtain

$$\|u\|_*^2 = \frac{4}{3}\big(\|\delta_x u\|^2 + \|\delta_y u\|^2\big) - \frac{1}{3}\big(\|\Delta_x u\|^2 + \|\Delta_y u\|^2\big) \ge \|\delta_x u\|^2 + \|\delta_y u\|^2.$$

The lemma is confirmed. □

Lemma 2.2. *The operators $\mathcal{A}_x$ and $\mathcal{A}_y$ are symmetric and positive semi-definite with respect to the inner product $(\cdot,\cdot)$ defined by (6).*

Proof. For any grid functions u, v defined on $\mathbf{\Omega}_h$, it follows from using the summation by parts and that

$$\begin{aligned}\big(\mathcal{A}_x u, v\big) =& \frac{4}{3}h_1 h_2 \sum_{i=0}^{M_1-1} \Big[\frac{1}{2}\delta_x u_{i+\frac{1}{2},0}\delta_x v_{i+\frac{1}{2},0} + \sum_{j=1}^{M_2-1} \delta_x u_{i+\frac{1}{2},j}\delta_x v_{i+\frac{1}{2},j} \\ &+ \frac{1}{2}\delta_x u_{i+\frac{1}{2},M_2}\delta_x v_{i+\frac{1}{2},M_2}\Big] - \frac{1}{3}h_1 h_2 \sum_{i=1}^{M_1-1} \Big[\frac{1}{2}\Delta_x u_{i,0}\Delta_x v_{i,0} \\ &+ \sum_{j=1}^{M_2-1} \Delta_x u_{i,j}\Delta_x v_{i,j} + \frac{1}{2}\Delta_x u_{i,M_2}\Delta_x v_{i,M_2}\Big] \\ =& \big(u, \mathcal{A}_x v\big),\end{aligned}$$

and

$$\begin{aligned}\big(\mathcal{A}_x u, u\big) =& \frac{4}{3}h_1 h_2 \sum_{i=0}^{M_1-1} \Big[\frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},0}\big)^2 + \sum_{j=1}^{M_2-1} \big(\delta_x u_{i+\frac{1}{2},j}\big)^2 + \frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},M_2}\big)^2\Big] \\ &- \frac{1}{3}h_1 h_2 \sum_{i=1}^{M_1-1} \Big[\frac{1}{2}\big(\Delta_x u_{i,0}\big)^2 + \sum_{j=1}^{M_2-1} \big(\Delta_x u_{i,j}\big)^2 + \frac{1}{2}\big(\Delta_x u_{i,M_2}\big)^2\Big] \\ =& \frac{4}{3}\|\delta_x u\|^2 - \frac{1}{3}\|\Delta_x u\|^2 \geq \|\delta_x u\|^2 \geq 0.\end{aligned}$$

Likewise, it can be verified that

$$\big(\mathcal{A}_y u, v\big) = \big(u, \mathcal{A}_y v\big) \quad \text{and} \quad \big(\mathcal{A}_y u, u\big) \geq \frac{4}{3}\|\delta_y u\|^2 - \frac{1}{3}\|\Delta_y u\|^2 \geq \|\delta_y u\|^2 \geq 0.$$

Hence, the conclusions of the lemma are true. □

Using the five lemmas stated in the paper [25], we will conclude that the difference operators $\mathcal{A}_x$ and $\mathcal{A}_y$ are important to the construction of the fourth-order discretisation for the second-order derivative in all the spatial grid points. Actually, the following lemma is the promotion of the five lemmas stated in the paper [25]. It is easy to verify the conclusion of the lemma by using the Taylor expansion with integral residual items.

Lemma 2.3. *Suppose that* $\omega(x, y) \in C^{6,6}\big([x_l, y_r] \times [y_d, y_u]\big)$ *satisfies the following conditions*

$$\partial_x^k \omega(x_l, y) = \partial_x^k \omega(x_r, y) = 0, \quad \partial_y^k \omega(x, y_d) = \partial_y^k \omega(x, y_u) = 0, \quad k = 1, 3, 5. \tag{9}$$

We then have

$$\partial_x^2 \omega(x_i, y) = -\mathcal{A}_x \omega(x_i, y) + \mathcal{R}_i(y), \quad 0 \leq i \leq M_1, \forall y \in [y_d, y_u], \tag{10}$$

and

$$\partial_y^2 \omega(x, y_j) = -\mathcal{A}_y \omega(x, y_j) + \mathcal{R}_j(x), \quad 0 \leq j \leq M_2, \forall x \in [x_l, y_r], \tag{11}$$

where the residuals $\mathcal{R}_i(y)$ *and* $\mathcal{R}_j(x)$ *satisfy the following approximations*

$$\mathcal{R}_i(y) = \mathcal{O}(h_1^4) \quad \text{and} \quad \mathcal{R}_j(x) = \mathcal{O}(h_2^4).$$

Proof. Following the five lemmas given in the paper [25], we obtain

$$\partial_x^2\omega(x_i,y)=\begin{cases}\dfrac{7}{3h_1}\delta_x\omega(x_{\frac12},y)-\dfrac16\delta_x^2\omega(x_1,y)+\mathcal{R}_0(y), \quad i=0,\\ -\dfrac{1}{6h_1}\delta_x\omega(x_{\frac12},y)+\dfrac76\delta_x^2\omega(x_1,y)-\dfrac{1}{12}\delta_x^2\omega(x_2,y)+\mathcal{R}_1(y), \quad i=1,\\ \dfrac43\delta_x^2\omega(x_i,y)-\dfrac13\Delta_x^2\omega(x_i,y)+\mathcal{R}_i(y), \quad 2\le i\le M_1-2,\\ \dfrac{1}{6h_1}\delta_x\omega(x_{M_1-\frac12},y)+\dfrac76\delta_x^2\omega(x_{M_1-1},y)-\dfrac{1}{12}\delta_x^2\omega(x_{M_1-2},y)\\ \qquad\qquad+\mathcal{R}_{M-1}(y), \quad i=M_1-1,\\ -\dfrac{7}{3h_1}\delta_x\omega(x_{M_1-\frac12},y)-\dfrac16\delta_x^2\omega(x_{M_1-1},y)+\mathcal{R}_{M_1}(y), \quad i=M_1,\end{cases}$$

i.e.,

$$\partial_x^2\omega(x_i,y)=-\mathcal{A}_x\omega(x_i,y)+\mathcal{R}_i(y), \quad 0\le i\le M_1,\ \forall y\in[y_d,y_u],$$

and there exists a positive constant C_1 such that

$$|\mathcal{R}_i(y)|\le C_1h_1^4.$$

Similarly, we also have

$$\partial_y^2\omega(x,y_j)=-\mathcal{A}_y\omega(x,y_j)+\mathcal{R}_j(x), \quad 0\le j\le M_2,\ \forall x\in[x_l,x_r],$$

and there exists a positive constant C_2 such that

$$|\mathcal{R}_j(x)|\le C_2h_2^4.$$

The conclusions of the lemma have been proved. □

2.2. Fourth-order spatial semidiscretisation, stability and convergence. It can be obtained straightforwardly from the Hamiltonian wave equation (1) that

$$\begin{aligned} a^2u_{xx}&=u_{tt}-a^2u_{yy}-f(u),\\ a^2u_x^{(3)}&=u_{ttx}-a^2u_{xyy}-f'(u)u_x,\\ a^2u_x^{(4)}&=u_{ttxx}-a^2u_{xxyy}-f''(u)u_x^2-f'(u)u_{xx},\\ a^2u_x^{(5)}&=u_{ttxxx}-a^2u_{xxxxyy}-f'''(u)u_x^3-3f''(u)u_{xx}u_x-f'(u)u_x^{(3)}.\end{aligned} \tag{12}$$

Therefore, the boundary conditions (2) deliver

$$u_x^{(3)}|_{x_l}=0, \quad u_x^{(3)}|_{x_r}=0, \quad u_x^{(5)}|_{x_l}=0, \quad u_x^{(5)}|_{x_r}=0, \quad y_d\le y\le y_u, \quad t_0<t\le T. \tag{13}$$

In a similar way, we also have

$$u_y^{(3)}|_{y_d}=0, \quad u_y^{(3)}|_{y_u}=0, \quad u_y^{(5)}|_{y_d}=0, \quad u_y^{(5)}|_{y_u}=0, \quad x_l\le x\le x_r, \quad t_0<t\le T. \tag{14}$$

Under the assumption of $u(x,y,t)\in C^{6,6,2}\Big(\bar{\mathbf{\Omega}}\times[t_0,T]\Big)$, and from the equations (13), (14) and the Lemma 2.3, we dispose the spatial derivatives of the Hamiltonian systems (1)-(2) and arrive at the following fourth-order semi-discrete scheme

$$\begin{aligned} U_{ij}''(t)+a^2\Big(\mathcal{A}_xU_{ij}(t)+\mathcal{A}_yU_{ij}(t)\Big)&=f\big(U_{ij}(t)\big)+\mathcal{R}_{ij}(t),\\ &0\le i\le M_1,\ 0\le j\le M_2,\ t_0\le t\le T,\end{aligned} \tag{15}$$

where $U_{ij}(t)$ represent the exact solutions $u(x,y,t)$ on the spatial grid $\mathbf{\Omega}_h\times[t_0,T]$, and the residuals $\mathcal{R}_{ij}(t)$ satisfy

$$\mathcal{R}_{ij}(t)=\mathcal{O}(h_1^4+h_2^4), \quad 0\le i\le M_1,\ 0\le j\le M_2,\ t_0\le t\le T.$$

Omitting the residuals $\mathcal{R}_{ij}(t)$ in (15) and using $u_{ij}(t) \approx U(x_i, y_j, t)$ result in the following semi-discrete scheme

$$\begin{aligned} u''_{ij}(t) + a^2\big(\mathcal{A}_x u_{ij}(t) + \mathcal{A}_y u_{ij}(t)\big) &= f\big(u_{ij}(t)\big), \\ 0 \le i \le M_1,\ 0 \le j \le M_2,\ t_0 &\le t \le T. \end{aligned} \tag{16}$$

Let $u(t) = \{u_{ij}(t) \mid (x_i, y_j) \in \mathbf{\Omega}_h\}$. Then the equations in (16) can be rewritten in a compact form as follows:

$$u''(t) + a^2\big(\mathcal{A}_x u(t) + \mathcal{A}_y u(t)\big) = f\big(u(t)\big), \quad t_0 \le t \le T. \tag{17}$$

With the semi-discrete scheme (16), we have the following energy conservation law.

Theorem 2.1. *Suppose that $u(t) = \{u_{ij}(t) \mid (x_i, y_j) \in \mathbf{\Omega}_h\}$ is the solution of the semi-discrete scheme (16) or (17). We then have the following discrete energy conservation law:*

$$E(t) \equiv \frac{1}{2}\|u'(t)\|^2 + \frac{a^2}{2}\|u(t)\|_*^2 + \tilde{V}(u(t)) = E(t_0), \tag{18}$$

where the potential function $\tilde{V}\big(u(t)\big)$ is given by

(19)
$$\begin{aligned} \tilde{V}\big(u(t)\big) =& h_1 h_2 \sum_{i=1}^{M_1-1}\sum_{j=1}^{M_2-1} V\big(u_{ij}(t)\big) + \frac{h_1 h_2}{4}\Big[V\big(u_{0,0}(t)\big) + V\big(u_{M_1,0}(t)\big) \\ &+ V\big(u_{0,M_2}(t)\big) + V\big(u_{M_1,M_2}(t)\big)\Big] + \frac{h_1 h_2}{2}\sum_{i=1}^{M_1-1}\Big[V\big(u_{i,0}(t)\big) + V\big(u_{i,M_2}(t)\big)\Big] \\ &+ \frac{h_1 h_2}{2}\sum_{j=1}^{M_2-1}\Big[V\big(u_{0,j}(t)\big) + V\big(u_{M_1,j}(t)\big)\Big]. \end{aligned}$$

Proof. Taking the inner product of (17) with $u'(t)$ and following careful calculations, we have

$$\Big(u''(t), u'(t)\Big) + a^2\Big[\Big(\mathcal{A}_x u(t), u'(t)\Big) + \Big(\mathcal{A}_y u(t), u'(t)\Big)\Big] - \Big(f\big(u(t)\big), u'(t)\Big) = 0, \tag{20}$$

where

(21)
$$\begin{aligned} \Big(u''(t), u'(t)\Big) =& \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\bigg\{\frac{h_1 h_2}{4}\Big[\big(u'_{0,0}(t)\big)^2 + \big(u'_{M_1,0}(t)\big)^2 + \big(u'_{0,M_2}(t)\big)^2 + \big(u'_{M_1,M_2}(t)\big)^2\Big] \\ &+ \frac{h_1 h_2}{2}\sum_{i=1}^{M_1-1}\Big[\big(u'_{i,0}(t)\big)^2 + \big(u'_{i,M_2}(t)\big)^2\Big] \\ &+ \frac{h_1 h_2}{2}\sum_{j=1}^{M_2-1}\Big[\big(u'_{0,j}(t)\big)^2 + \big(u'_{M_1,j}\big)^2\Big] \\ &+ h_1 h_2 \sum_{i=1}^{M_1-1}\sum_{j=1}^{M_2-1}\big(u'_{ij}(t)\big)^2\bigg\} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(u'(t), u'(t)\Big) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u'(t)\|^2, \end{aligned}$$

(22)

$$
\begin{aligned}
&a^2\Big[\Big(\mathcal{A}_x u(t), u'(t)\Big)+\Big(\mathcal{A}_y u(t), u'(t)\Big)\Big]\\
=&\frac{a^2}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Bigg\{\frac{4}{3}h_1h_2\sum_{i=0}^{M_1-1}\Big[\frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},0}(t)\big)^2+\sum_{j=1}^{M_2-1}\big(\delta_x u_{i+\frac{1}{2},j}(t)\big)^2+\frac{1}{2}\big(\delta_x u_{i+\frac{1}{2},M_2}(t)\big)^2\Big]\\
&-\frac{1}{3}h_1h_2\sum_{i=1}^{M_1-1}\Big[\frac{1}{2}\big(\Delta_x u_{i,0}(t)\big)^2+\sum_{j=1}^{M_2-1}\big(\Delta_x u_{i,j}(t)\big)^2+\frac{1}{2}\big(\Delta_x u_{i,M_2}(t)\big)^2\Big]\\
&+\frac{4}{3}h_1h_2\sum_{j=0}^{M_2-1}\Big[\frac{1}{2}\big(\delta_y u_{0,j+\frac{1}{2}}(t)\big)^2+\sum_{i=1}^{M_1-1}\big(\delta_y u_{i,j+\frac{1}{2}}(t)\big)^2+\frac{1}{2}\big(\delta_y u_{M_1,j+\frac{1}{2}}(t)\big)^2\Big]\\
&-\frac{1}{3}h_1h_2\sum_{j=1}^{M_2-1}\Big[\frac{1}{2}\big(\Delta_y u_{0,j}(t)\big)^2+\sum_{i=1}^{M_1-1}\big(\Delta_y u_{i,j}(t)\big)^2+\frac{1}{2}\big(\Delta_x u_{M_1,j}(t)\big)^2\Big]\Bigg\}\\
=&\frac{a^2}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{4}{3}\big(\|\delta_x u(t)\|^2+\|\delta_y u(t)\|^2\big)-\frac{1}{3}\big(\|\Delta_x u(t)\|^2+\|\Delta_y u(t)\|^2\big)\Big]=\frac{a^2}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|_*^2,
\end{aligned}
$$

and

$$
\begin{aligned}
\Big(f\big(u(t)\big), u'(t)\Big)=&-\frac{\mathrm{d}}{\mathrm{d}t}\Bigg\{\frac{h_1h_2}{4}\Big[V\big(u_{0,0}(t)\big)+V\big(u_{M_1,0}(t)\big)\\
&+V\big(u_{0,M_2}(t)\big)+V\big(u_{M_1,M_2}(t)\big)\Big]\\
&+\frac{h_1h_2}{2}\sum_{i=1}^{M_1-1}\Big[V\big(u_{i,0}(t)\big)+V\big(u_{i,M_2}(t)\big)\Big]\\
&+\frac{h_1h_2}{2}\sum_{j=1}^{M_2-1}\Big[V\big(u_{0,j}(t)\big)+V\big(u_{M_1,j}(t)\big)\Big]\\
&+h_1h_2\sum_{i=1}^{M_1-1}\sum_{j=1}^{M_2-1}V\big(u_{ij}(t)\big)\Bigg\}\triangleq-\frac{\mathrm{d}}{\mathrm{d}t}\tilde{V}\big(u(t)\big).
\end{aligned}
\tag{23}
$$

Inserting (21)-(23) into (20) yields

$$
\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{2}\|u'(t)\|^2+\frac{a^2}{2}\|u(t)\|_*^2+\tilde{V}(u(t))\Big)=0. \tag{24}
$$

Therefore, the energy conservation law is valid. □

Following the discrete energy conservation law (18) shown by Theorem 2.1, we can obtain the following result on stability analysis.

Theorem 2.2. *Assume that the potential function $V(\cdot)$ is positive and $u(t)=\{u_{ij}(t)\mid(x_i,y_j)\in\mathbf{\Omega}_h\}$ is the solution of the semi-discrete scheme* (16) *or* (17)*. Then the semi-discrete scheme is stable under the discrete H^1-norm, that is, there exists a constant C_3 such that*

$$
\|u(t)\|_{H^1}^2\le 2\|\varphi\|^2+C_3E(t_0), \tag{25}
$$

where $\|u(t)\|_{H^1}^2=\|u(t)\|^2+\|\delta_x u(t)\|^2+\|\delta_y u(t)\|^2$.

Proof. According to the discrete energy conservation law (18) and Lemma 2.1, we have

$$\|u'(t)\|^2 \leq 2E(t_0) \quad \text{and} \quad \|\delta_x u(t)\|^2 + \|\delta_y u(t)\|^2 \leq \frac{2}{a^2}E(t_0). \tag{26}$$

For any $t \geq t_0$, the Cauchy-Schwarz inequality yields

$$\begin{aligned} u_{ij}^2(t) &\leq 2u_{ij}^2(t_0) + 2\left(\int_{t_0}^t u'_{ij}(\zeta)\mathrm{d}\zeta\right)^2 \\ &\leq 2u_{ij}^2(t_0) + 2(t-t_0)\int_{t_0}^t u'^2_{ij}(\zeta)\mathrm{d}\zeta. \end{aligned} \tag{27}$$

Therefore, it follows from (27) that

$$\|u(t)\|^2 \leq 2\|u(t_0)\|^2 + 2(t-t_0)\int_{t_0}^t \|u'(\zeta)\|^2\mathrm{d}\zeta. \tag{28}$$

Combining the inequalities (26) and (28) conforms the conclusion of the theorem. □

Remark 2.1. *Since the potential function $V(\cdot)$ is only used through its gradient, any $V(\cdot)+c$ can fit for the equations with a suitable constant $c \geq 0$. Under this assumption that $V(\cdot)$ is positive, together with the discrete energy conservation law, we can prove the stability of the semi-discrete scheme.*

In what follows, we assume that the function $f(\cdot)$ satisfies a Lipschitz condition with respect to u, namely, there is a positive constant L, s.t.

$$\|f(u) - f(v)\| \leq L\|u - v\|, \quad \forall u, v. \tag{29}$$

We now quote the well-known Gronwall inequality summarised below, which will play an important role in the proof of the convergence for the semi-discrete scheme (16) or (17).

Lemma 2.4. *Suppose that $f(t), g(t)$ are two nonnegative functions defined on $[t_0, T]$, and satisfy the following differential inequality*

$$f'(t) \leq C_4 f(t) + g(t).$$

Then

$$f(t) \leq e^{C_4 t}\Big[f(t_0) + \int_{t_0}^t e^{-C_4 s}g(s)\mathrm{d}s\Big], \quad \forall t \in [t_0, T],$$

where C_4 is a nonnegative constant.

Theorem 2.3. *It is assumed that $u(x,y,t) \in C^{6,6,2}\Big(\bar{\mathbf{\Omega}} \times [t_0,T]\Big)$ is the solution of (1)-(2) and $u(t) = \{u_{ij}(t) \mid (x_i, y_j) \in \mathbf{\Omega}_h\}$ is the solution of the semi-discrete scheme (16) or (17). Then, we have*

$$\|e(t)\|_{H^1} = \mathcal{O}(h_1^4 + h_2^4), \quad \forall t \in [t_0, T], \tag{30}$$

where $e_{ij}(t) = U_{ij}(t) - u_{ij}(t)$, $0 \leq i \leq M_1, 0 \leq j \leq M_2$.

Proof. Subtracting (16) from (15), and noticing the initial conditions, we obtain the error system

$$\begin{cases} e''(t) + a^2\Big(\mathcal{A}_x e(t) + \mathcal{A}_y e(t)\Big) = f\big(U(t)\big) - f\big(u(t)\big) + \mathcal{R}(t), \quad t_0 \leq t \leq T, \\ e(t_0) = 0,\ e'(t_0) = 0, \end{cases}$$

where $\mathcal{R}(t) = \{\mathcal{R}_{ij}(t) \mid 0 \le i \le M_1, 0 \le j \le M_2\}$. Taking the inner product with $e'(t)$ yields

$$\begin{aligned}&\big(e''(t), e'(t)\big) + a^2 \left[\big(\mathcal{A}_x e(t), e'(t)\big) + \big(\mathcal{A}_y e(t), e'(t)\big)\right]\\ =&\Big(f\big(U(t)\big) - f\big(u(t)\big), e'(t)\Big) + \big(\mathcal{R}(t), e'(t)\big).\end{aligned}$$

A careful calculation gives

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|e'(t)\|^2 + a^2\|e(t)\|_*^2\Big) \le& L\|e(t)\| \cdot \|e'(t)\| + \|\mathcal{R}(t)\| \cdot \|e'(t)\|\\ \le& C_5\Big(\|e'(t)\|^2 + a^2\|e(t)\|_*^2\Big) + \frac{1}{2}\|\mathcal{R}(t)\|^2,\end{aligned}$$

i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|e'(t)\|^2 + a^2\|e(t)\|_*^2\Big) \le 2C_5\Big(\|e'(t)\|^2 + a^2\|e(t)\|_*^2\Big) + \|\mathcal{R}(t)\|^2,$$

where C_5 is a constant. Applying the Gronwall inequality to the above inequality with the exact initial conditions, we obtain

$$\|e'(t)\|^2 + a^2\|e(t)\|_*^2 \le \int_{t_0}^{t} \exp\big(2C_5(t-s)\big)\|\mathcal{R}(s)\|^2 \mathrm{d}s = \mathcal{O}(h_1^8 + h_2^8).$$

The estimations of $\|e'(t)\|^2$ and $\|e(t)\|_*^2$ can be yielded

$$\|e'(t)\|^2 = \mathcal{O}(h_1^8 + h_2^8) \quad \text{and} \quad \|e(t)\|_*^2 = \mathcal{O}(h_1^8 + h_2^8).$$

Similarly to the proof process of Theorem 2.2, we obtain

$$\|e(t)\|^2 \le 2\|e(t_0)\|^2 + 2(t-t_0)\int_{t_0}^{t} \|e'(\zeta)\|^2 \mathrm{d}\zeta.$$

On noticing that $e(t_0) = 0$, we have

$$\|e(t)\|^2 = \mathcal{O}(h_1^8 + h_2^8).$$

Using Lemma 2.1 to the estimation of $\|e(t)\|_*^2$ leads to

$$|e(t)|_1^2 = \|\delta_x e(t)\|^2 + \|\delta_y e(t)\|^2 = \mathcal{O}(h_1^8 + h_2^8).$$

Therefore, the error estimation under the H_1 semi-norm is obtained

$$\|e(t)\|_{H^1}^2 = \|e(t)\|^2 + \|\delta_x e(t)\|^2 + \|\delta_y e(t)\|^2 = \mathcal{O}(h_1^8 + h_2^8), \quad \forall t \in [t_0, T].$$

The conclusion of the theorem is confirmed. □

2.3. Corresponding Hamiltonian ODEs. Let $w_j(t) = \Big(u_{0,j}(t), u_{1,j}(t), \ldots, u_{M_1,j}(t)\Big)^{\mathsf{T}}$ and $f\big(w_j(t)\big) = \Big(f\big(u_{0,j}(t)\big), f\big(u_{1,j}(t)\big), \ldots, f\big(u_{M_1,j}(t)\big)\Big)^{\mathsf{T}}$, the semi-discrete scheme (16) or (17) is identical to the following nonlinear ODEs

$$\begin{cases} w''(t) + \dfrac{a^2}{12}\left(\dfrac{I_{M_2} \otimes D_{M_1}}{h_1^2} + \dfrac{D_{M_2} \otimes I_{M_1}}{h_2^2}\right) w(t) = f\big(w(t)\big), \quad t_0 < t \le T, \\ w(t_0) = \tilde{\varphi} = (\tilde{\varphi}_0, \ldots, \tilde{\varphi}_{M_2})^{\mathsf{T}}, \quad w'(t_0) = \tilde{\psi} = (\tilde{\psi}_0, \ldots, \tilde{\psi}_{M_2})^{\mathsf{T}}, \end{cases} \tag{31}$$

where I_d are $d \times d$ identity matrix with $d = M_1, M_2$, $\otimes$ is the Kronecker product, $w(t) = \big(w_0(t), \ldots, w_{M_2}(t)\big)^\intercal$,

$$D_d = \begin{pmatrix} 30 & -32 & 2 & & & & \\ -16 & 31 & -16 & 1 & & & \\ 1 & -16 & 30 & -16 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 1 & -16 & 30 & -16 & 1 \\ & & & 1 & -16 & 31 & -16 \\ & & & & 2 & -32 & 30 \end{pmatrix}_{d\times d},$$

and

$$f\big(w(t)\big) = \Big(f\big(w_0(t)\big), \ldots, f\big(w_{M_2}(t)\big)\Big)^\intercal,\ \tilde{\varphi}_j = \Big(\varphi(x_0, y_j), \ldots, \varphi(x_{M_1}, y_j)\Big)^\intercal,$$

$$\tilde{\psi}_j = \Big(\psi(x_0, y_j), \ldots, \psi(x_{M_1}, y_j)\Big)^\intercal.$$

Multiplying the system (31) with the matrix $A = h_1h_2A_{M_2} \otimes A_{M_1}$, we obtain

$$\begin{cases} Aw''(t) + Bw(t) = \tilde{f}\big(w(t)\big), & t_0 < t \le T, \\ w(t_0) = \tilde{\varphi}, \quad w'(t_0) = \tilde{\psi}, \end{cases} \tag{32}$$

which is equivalent to (31), where $A_d = \mathrm{diag}\big(\frac{1}{2}, 1, \ldots, 1, \frac{1}{2}\big)$ for $d = M_1$ and M_2, and $B = \frac{a^2}{12}A\left(\frac{I_{M_2}\otimes D_{M_1}}{h_1^2} + \frac{D_{M_2}\otimes I_{M_1}}{h_2^2}\right)$ is a positive semi-definite matrix, and $\tilde{f}\big(w(t)\big) = Af\big(w(t)\big)$ is the negative gradient of the energy potential function $\tilde{V}\big(w(t)\big)$ defined by (19). The system (32) is a Hamiltonian system with the Hamiltonian

$$H(w'(t), w(t)) = \frac{1}{2}w'(t)^\intercal Aw'(t) + \frac{1}{2}w(t)^\intercal Bw(t) + \tilde{V}\big(w(t)\big). \tag{33}$$

Theorem 2.4. *Assume that $u(t) = \{u_{ij}(t) \mid (x_i, y_j) \in \mathbf{\Omega}_h\}$ is the solution of the semi-discrete scheme* (16)*, or equivalently, the Hamiltonian system* (32)*. Then we have*

$$H\big(w'(t), w(t)\big) = E(t), \quad t_0 \le t \le T.$$

Proof. Following the formula (33) and through careful calculations, we obtain

$$\begin{aligned} H\big(w'(t), w(t)\big) &= \frac{1}{2}w'(t)^\intercal Aw'(t) + \frac{1}{2}w(t)^\intercal Bw(t) + \tilde{V}\big(w(t)\big) \\ &= \frac{1}{2}\|u'(t)\|^2 + \frac{a^2}{2}\|u(t)\|_*^2 + \tilde{V}\big(u(t)\big) \\ &= E(t). \end{aligned}$$

The conclusion of the theorem is proved. □

3. Envergy-preserving time integrators: AVF formula

In this section, we concentrate on constructing energy-conservation time integrators for the following nonlinear Hamiltonian system of ODEs

$$\begin{cases} Aw''(t) + Bw(t) = \tilde{f}\big(w(t)\big), & t_0 < t \le T, \\ w(t_0) = \tilde{\varphi}, \quad w'(t_0) = \tilde{\psi}. \end{cases} \tag{34}$$

Let $q(t) = w(t), p(t) = Aq'(t)$. Then the system (34) can be expressed as the following first-order Hamiltonian system of ODEs

$$\begin{cases} p'(t) = -\nabla_q H(p, q), \\ q'(t) = \nabla_p H(p, q), \end{cases} \tag{35}$$

with the initial values $p(t_0) = A\tilde{\psi},\ q(t_0) = \tilde{\varphi}$ and the Hamiltonian

$$H(p, q) = \frac{1}{2}p^{\intercal}A^{-1}p + \frac{1}{2}q^{\intercal}Bq + \tilde{V}(q), \tag{36}$$

which is identical to the following Hamiltonian

$$H\big(w'(t), w(t)\big) = \frac{1}{2}w'(t)^{\intercal}Aw'(t) + \frac{1}{2}w(t)^{\intercal}Bw(t) + \tilde{V}\big(w(t)\big). \tag{37}$$

The energy conservation is one of the essential properties of the Hamiltonian system, whose Hamiltonians can be regarded as the approximate energy of the original PDEs. Therefore, it is of great importance to construct energy-conservation time integrators (see, e.g. [4, 7, 10, 18, 19, 27, 32, 36, 39, 40]). For instance, we consider the following Hamiltonian system

$$\dot{z} = J^{-1}\nabla H(z), \tag{38}$$

where J is a skew-symmetric matrix with the form

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{39}$$

and H is the Hamiltonian. McLachlan et al. derived the AVF formula in [32], i.e.,

$$z_{n+1} = z_n + \tau \int_0^1 J^{-1}\nabla H\big((1-s)z_n + sz_{n+1}\big)\mathrm{d}s. \tag{40}$$

The Hamiltonian of the system (38) can be preserved exactly by the AVF formula (40).

Applying the AVF formula (40) to Hamiltonian system (35) with a straightforward calculation, we obtain

$$\begin{cases} q^{n+1} = q^n + \tau A^{-1}p^n + \dfrac{\tau^2}{2}A^{-1}\displaystyle\int_0^1 g\big((1-s)q^n + sq^{n+1}\big)\mathrm{d}s, \\ p^{n+1} = p^n + \tau \displaystyle\int_0^1 g\big((1-s)q^n + sq^{n+1}\big)\mathrm{d}s, \end{cases} \tag{41}$$

which can preserve the energy (or Hamiltonian) of the system (34) exactly, namely,

$$H(w'^{n+1}, w^{n+1}) = H(w'^n, w^n),$$

where $g(w) = -Bw + \tilde{f}(w)$ and $t_{n+1} = t_n + \tau$ with τ is the time stepsize. Let $q^n = w^n$ and $p^n = Aw'^n$. Then, the formula (41) is identical to

$$\begin{cases} w^{n+1} = w^n + \tau w'^n + \dfrac{\tau^2}{2}A^{-1}\displaystyle\int_0^1 g\big((1-s)w^n + sw^{n+1}\big)\mathrm{d}s, \\ w'^{n+1} = w'^n + \tau A^{-1}\displaystyle\int_0^1 g\big((1-s)w^n + sw^{n+1}\big)\mathrm{d}s. \end{cases} \tag{42}$$

Since $g(w) = -Bw + \tilde{f}(w)$, we can simplify the integral appeared in the formula (41) or (42) as

$$I_g = \int_0^1 g\big((1-s)w^n + sw^{n+1}\big)\mathrm{d}s = -\frac{1}{2}B\big(w^n + w^{n+1}\big) + \int_0^1 \tilde{f}\big((1-s)w^n + sw^{n+1}\big)\mathrm{d}s,$$

where $\tilde{f}(w) = Af(w)$ and $f(w) = \Big(f\big(w_0\big), \dots, f\big(w_{M_2}\big)\Big)^{\intercal}$ with $f(w_j) = \Big(f\big(u_{0,j}\big), f\big(u_{1,j}\big), \dots, f\big(u_{M_1,j}\big)\Big)^{\intercal}$. Moreover, from the fact that the function $f(u)$ satisfies

$f(u) = -\frac{\mathrm{d}V(u)}{\mathrm{d}u}$, we have

$$\int_0^1 f\big((1-s)u_{ij}^n + su_{ij}^{n+1}\big)\mathrm{d}s = -\frac{V(u_{ij}^{n+1}) - V(u_{ij}^n)}{u_{ij}^{n+1} - u_{ij}^n}.$$

Here, it should be noted that, if $u_{ij}^{n+1} = u_{ij}^n$, $0 \le i \le M_1, 0 \le j \le M_2$, then $\frac{V(u_{ij}^{n+1})-V(u_{ij}^n)}{u_{ij}^{n+1}-u_{ij}^n}$ is $\frac{0}{0}$, which can be understood as

$$\frac{V(u_{ij}^{n+1}) - V(u_{ij}^n)}{u_{ij}^{n+1} - u_{ij}^n} = \frac{\mathrm{d}V(u_{ij}^n)}{\mathrm{d}u} = -f(u_{ij}^n).$$

Therefore, the nonlinear integral $\displaystyle\int_0^1 \tilde{f}\big((1-s)w^n + sw^{n+1}\big)\mathrm{d}s$ can be expressed as:

$$\begin{aligned} &\int_0^1 \tilde{f}\big((1-s)w^n + sw^{n+1}\big)\mathrm{d}s \\ &= -A\frac{V(w^{n+1}) - V(w^n)}{w^{n+1} - w^n} \qquad (43)\\ &= -A\left(\frac{V(w_0^{n+1}) - V(w_0^n)}{w_0^{n+1} - w_0^n}, \frac{V(w_1^{n+1}) - V(w_1^n)}{w_1^{n+1} - w_1^n}, \dots, \frac{V(w_{M_2}^{n+1}) - V(w_{M_2}^n)}{w_{M_2}^{n+1} - w_{M_2}^n}\right)^\intercal \end{aligned}$$

with

$$\begin{aligned} &\frac{V(w_j^{n+1}) - V(w_j^n)}{w_1^{n+1} - w_j^n} \qquad (44)\\ &= \left(\frac{V(u_{0,j}^{n+1}) - V(u_{0,j}^n)}{u_{0,j}^{n+1} - u_{0,j}^n}, \frac{V(u_{1,j}^{n+1}) - V(u_{1,j}^n)}{u_{1,j}^{n+1} - u_{1,j}^n}, \dots, \frac{V(u_{M_1,j}^{n+1}) - V(u_{M_1,j}^n)}{u_{M_1,j}^{n+1} - u_{M_1,j}^n}\right)^\intercal \end{aligned}$$

According to the above analysis, we are now in a position to present the energy-conservation time integrator for the oscillatory Hamiltonian ODEs' system (34).

Theorem 3.1. *The following modified AVF formula*

$$\begin{cases} w^{n+1} = w^n + \tau w'^n - \dfrac{\tau^2}{4}A^{-1}B(w^n + w^{n+1}) - \dfrac{\tau^2}{2}\dfrac{V(w^{n+1}) - V(w^n)}{w^{n+1} - w^n}, \\ w'^{n+1} = w'^n - \dfrac{\tau}{2}A^{-1}B(w^n + w^{n+1}) - \tau\dfrac{V(w^{n+1}) - V(w^n)}{w^{n+1} - w^n}. \end{cases} \qquad (45)$$

for the Hamiltonian system of ODEs (34) *can preserve the energy* (37) *exactly:*

$$H(w'^{n+1}, w^{n+1}) = H(w'^n, w^n).$$

Here, $\frac{V(w^{n+1})-V(w^n)}{w^{n+1}-w^n}$ *is denoted by* (43) *and* (44)*.*

Remark 3.1. *Actually, the modified AVF formula* (45) *is a kind of discrete gradient, which is called the mean value discrete gradient and is a second-order approximation to the gradient* $\nabla\tilde{V}$ *of the energy potential function* (19) *at the midpoint of* w^n *and* w^{n+1} *(see, e.g.* [21, 41]*).*

Moreover, the symmetry of a method is also an essential property in long time integration. The definition of symmetry is given below (see [40, 41]).

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

According to the definition of symmetry, it can be verified that the modified AVF formula (45) is unaltered by exchanging $n+1 \leftrightarrow n$ and $\tau \leftrightarrow -\tau$. Therefore, the modified AVF formula (45) can be verified to be symmetric. In addition, the modified AVF formula (45) can be interpreted as the second-order mean value discrete gradient (see [21, 41]). Therefore, it is easy to clarify that the global error accuracy of the modified AVF formula (45) is second-order. In the following theorem, we show the symmetry and the global error accuracy of the modified AVF formula (45) for solving the resulting semi-discrete scheme (34).

Theorem 3.2. *The modified AVF formula* (45) *for the semi-discrete Hamiltonian ODEs' system* (34) *is symmetric with respect to the time variable and convergent of order two.*

Proof. The symmetry of the modified AVF formula (45) can be confirmed by exchanging $n+1 \leftrightarrow n$ and $\tau \leftrightarrow -\tau$, and we skip the detailed proof process. Since the modified AVF formula (45) is the second-order mean value discrete gradient (see [21]), the modified AVF formula (45) is convergent of order two. □

From the above analysis, it is clear that we have derived an energy-conservation fully discrete scheme for solving the two-dimensional Hamiltonian wave equations (1)-(2) by discreting the spatial derivatives of the PDEs via the fourth-order finite difference method and applying the AVF approach to the resulted Hamiltonian system of ODEs. Since the convergence order of the modified AVF method is $\mathcal{O}(\tau^2)$, the global error accuracy of the fully discrete scheme can get to $\mathcal{O}(\tau^2 + h_1^4 + h_2^4)$.

4. Numerical experiments

As stated in the introduction of this paper, the energy conservation law is an essential property for the two-dimensional Hamiltonian wave equations (1)-(2). The conserved quantities of the constructed numerical scheme can be used to evaluate the stability of the numerical schemes. In what follows, we will apply the derived energy-conservation scheme to three practical problems to verify the numerical accuracy and the numerical behaviour of energy preservation. For comparison, the time integrators we selected are:

- HBVM(5,1): the energy-preserving Hamiltonian Boundary Value Method of order two given in [6, 7].
- SV: the symplectic Störmer-Verlet formula of order two given in [20];

As is known, iterative solutions are required for implicit schemes. We use fixed-point iteration for the modified AVF formula (45) and the HBVM(5,1) method. We set the error tolerance as 10^{-15} for each time-step iteration procedure and set the maximum number of iterations to be 10.

4.1. Test problem: linear wave equation. In order to observe the accuracy of the spatial discretisation, we consider the following linear wave equation in two dimensions

$$u_{tt} - (u_{xx} + u_{yy}) = (1 + 2\pi^2)u, \tag{46}$$

over the region $(x, y) \in [-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}]$ with the initial conditions

$$u(x, y, 0) = \sin(\pi x)\sin(\pi y), \quad u_t(x, y, 0) = -\sin(\pi x)\sin(\pi y). \tag{47}$$

The exact solution of the problem is

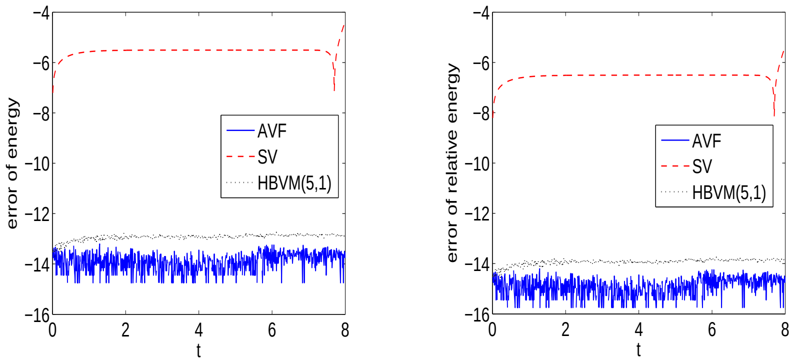
$$u(x, y, t) = e^{-t}\sin(\pi x)\sin(\pi y). \tag{48}$$

Obviously, the problem satisfies the homogenous Neumann boundary conditions. We compute the problem using the energy-conservation scheme proposed in this paper with fixed time stepsize $\tau = 0.001$ and several spatial steps (h_1, h_2) at time $T = 1$. The numerical results in Table 1 demonstrate that the spatial discretisation converges with order four under the l_2-norm, H^1-norm and l_∞-norm.

TABLE 1. The convergence order in space of numerical solutions at $T = 1$ with different spatial steps (h_1, h_2) and sufficiently small time stepsize $\tau = 0.001$ correspond to different norms.

(h_1, h_2)	l_2-norm		H^1-norm		l_∞-norm	
	$\Vert u^n - U^n\Vert_2$	order	$\Vert u^n - U^n\Vert_{H^1}$	order	$\Vert u^n - U^n\Vert_\infty$	order
$(\frac{1}{10}, \frac{1}{10})$	0.000427480135620	*	0.001891443502178	*	0.000854960271242	*
$(\frac{1}{20}, \frac{1}{20})$	0.000026875366806	3.9915	0.000119281389067	3.9870	0.000053750733614	3.9915
$(\frac{1}{40}, \frac{1}{40})$	0.000001668099766	4.0100	0.000007409267309	4.0089	0.000003336199529	4.0100
$(\frac{1}{80}, \frac{1}{80})$	0.000000089928878	4.2133	0.000000399517803	4.2130	0.000000179857733	4.2133

We then choose the stepsizes $h_1 = h_2 = 0.025$ and $\tau = 0.01$ for solving the problem and illustrate the conservative property of the new scheme in Fig. 1. The logarithms of the discrete energy error $|E(t_n) - E(t_0)|$ and the relative discrete energy error $|E(t_n) - E(t_0)|/E(t_0)$ are plotted in Fig. 1 (a) and (b), respectively. It can be observed that the energy obtained by the new scheme is well conserved.



(a) $|E(t_n) - E(t_0)|$ (b) $|E(t_n) - E(t_0)|/E(t_0)$

FIGURE 1. The logarithms of the discrete energy error (a) and the relative discrete energy error (b).

4.2. Simulation of two-dimensional sine-Gordon equations. In this subsection, the proposed new energy-conservation scheme is applied to simulate the two-dimensional sine-Gordon equation:

$$u_{tt} - (u_{xx} + u_{yy}) = -\sin(u), \quad 0 < t \le T, \tag{49}$$

over the region $\Omega = [-a, a]\times[-b, b]$. The problem is equipped with the homogeneous Neumann boundary conditions

$$u_x(\pm a, y, t) = u_y(x, \pm b, t) = 0, \tag{50}$$

and the initial conditions

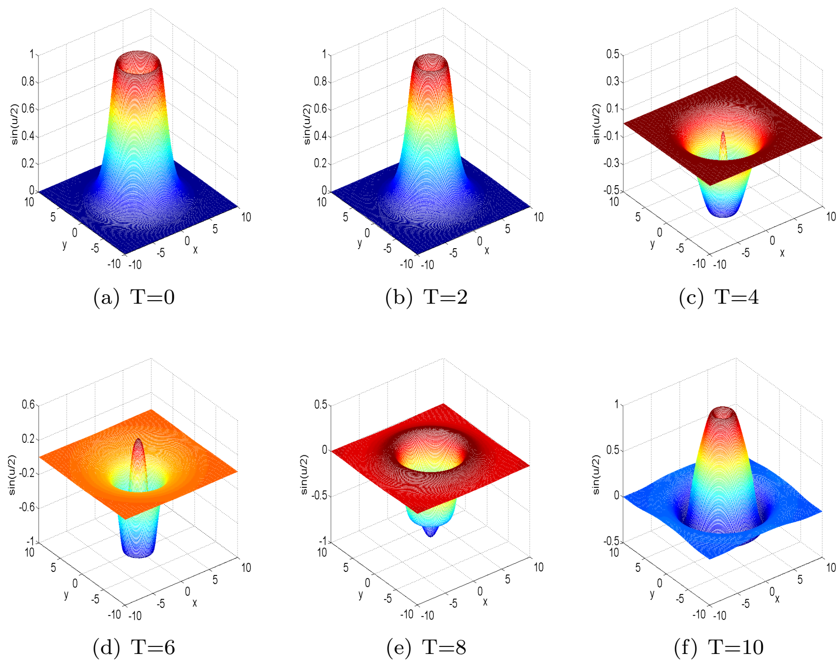
$$u(x, y, 0) = f(x, y), \quad u_t(x, y, 0) = g(x, y). \tag{51}$$

In general, the exact solution of the 2D sine-Gordon equation cannot be obtained exactly. Therefore, the conservative property of the energy becomes significant to examine the superiority of a numerical approach. Moreover, it has been known that different initial conditions will lead to different numerical phenomena. In what follows, we will use the new scheme to simulate two kinds of particular circular ring solitons. The initial conditions and parameters are chosen similarly to those in [5, 38].

Problem 1. *(Circular ring soliton)* We choose the initial conditions as:

$$f(x,y) = 4\arctan\Big(\exp\big(3-\sqrt{x^2+y^2}\big)\Big), \quad g(x,y)=0, \tag{52}$$

over the two-dimensional domain $(x,y) \in [-10,10]\times[-10,10]$. We simulate the problem by using the spatial steps $h_1 = h_2 = 0.2$ and time step $\tau = 0.01$. The simulation results and the corresponding contours at times $t = 0, 2, 4, 6, 8, 10$ in terms of $\sin(u/2)$ are plotted in Fig. 2 and Fig. 3, respectively. The conservative behaviour of the new scheme is shown in Fig. 4 from which it can be observed that the energy is well conserved. In comparison with the classical SV method and the HBVM(5,1) method, the modified AVF method (45) has superior property of energy conservation.



(a) T=0 (b) T=2 (c) T=4

(d) T=6 (e) T=8 (f) T=10

FIGURE 2. Circular ring solitons: the function of $\sin(u/2)$ for the numerical solutions at times $t = 0, 2, 4, 6, 8$ and 10.

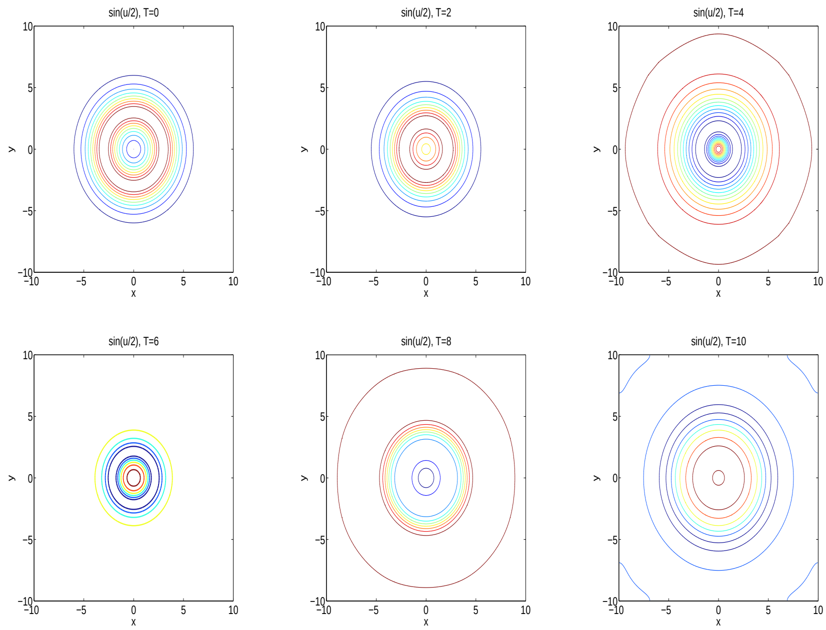
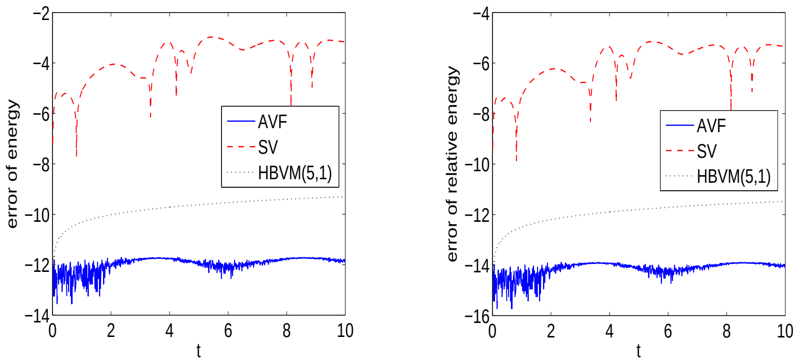


FIGURE 3. Circular ring solitons: contours of $\sin(u/2)$ for the numerical solutions at times $t = 0, 2, 4, 6, 8$ and 10.



(a) $|E(t_n) - E(t_0)|$ (b) $|E(t_n) - E(t_0)|/E(t_0)$

FIGURE 4. The logarithms of the discrete energy error (a) and the relative discrete energy error (b).

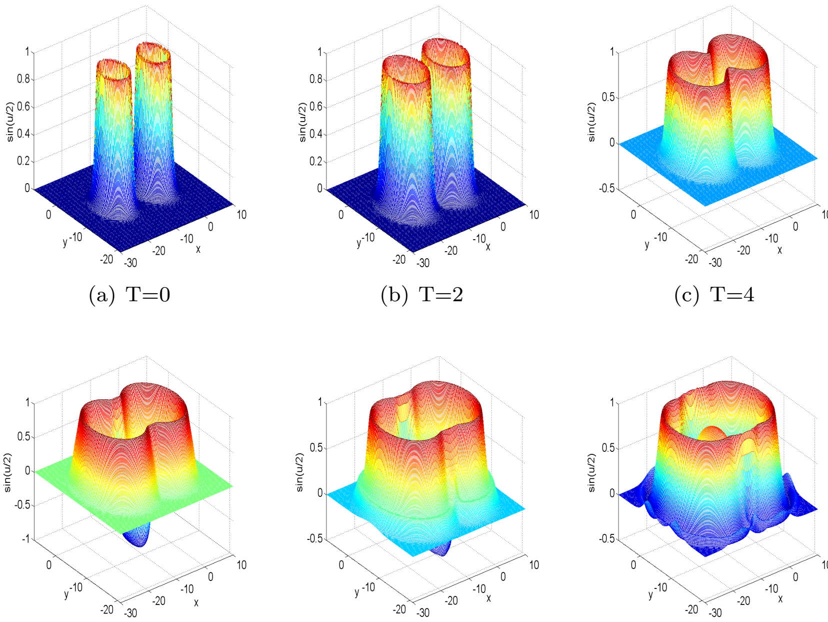
Problem 2. *(The collision of two circular solitons)* Furthermore, we take the following initial conditions:

(53)

$$f(x, y) = 4\arctan\Big(\exp\Big(\frac{4 - \sqrt{(x+3)^2 + (y+7)^2}}{0.436}\Big)\Big), \ -10 \le x \le 10, \ -7 \le y \le 7,$$

$$g(x, y) = 4.13\text{sech}\Big(\exp\Big(\frac{4 - \sqrt{(x+3)^2 + (y+7)^2}}{0.436}\Big)\Big), \ -10 \le x \le 10, \ -7 \le y \le 7,$$

and expand the solution across the sides $x = -10$ and $y = -7$ using the symmetry properties of the problem. We try to seek the solutions over the domain $(x, y) \in [-30, 10] \times [-21, 7]$ with the spatial steps $h_1 = 0.4, h_2 = 0.28$ and time step $\tau = 0.01$. The simulating results and the corresponding contour maps in terms of $\sin(u/2)$ at times $t = 0, 2, 4, 6, 8, 10$ are depicted in Fig.5 and Fig.6, respectively. The numerical results show the collision between two expanding circular ring solitons. The conservative behaviour of the discrete energy is demonstrated in Fig. 7. It again show that the modified AVF method (45) is more advantageous to the classical SV method and the HBVM(5,1) method.



(a) T=0 (b) T=2 (c) T=4

(d) T=6 (e) T=8 (f) T=10

FIGURE 5. Circular of two ring solitons: the function of $\sin(u/2)$ for the numerical solutions at times $t = 0, 2, 4, 6, 8$ and 10.

5. Conclusions

In this paper, incorporating the fourth-order finite difference method and the AVF approach, we derived and analysed a novel energy-conservation scheme for the two-dimensional Hamiltonian wave equations with the homogenous Neumann boundary conditions. In this work, we first analysed some properties of the fourth-order finite difference operators and proposed the spatial semi-discrete scheme. The energy conservation law, the stability and the convergence of the finite difference scheme were analysed in detail. Moreover, the semi-discrete scheme can be expressed as the particular Hamiltonian system of ODEs (34), and its Hamiltonian (37) is equivalent to the discrete energy (18). For the time integration, the AVF approach is applied to preserve the Hamiltonian of the system (34) obtained from the spatial discretisation. The perfect combination of the fourth-order finite difference method and the AVF approach yields a novel and efficient numerical scheme

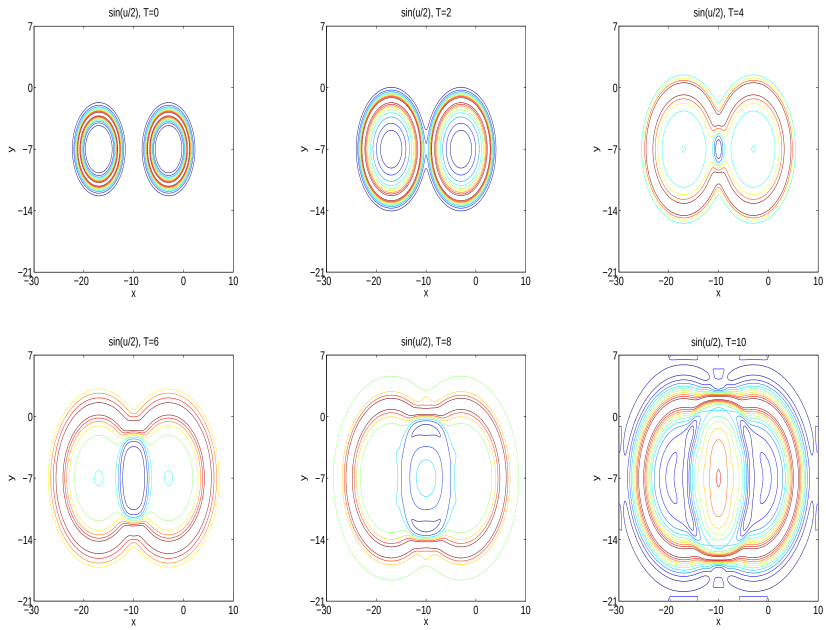
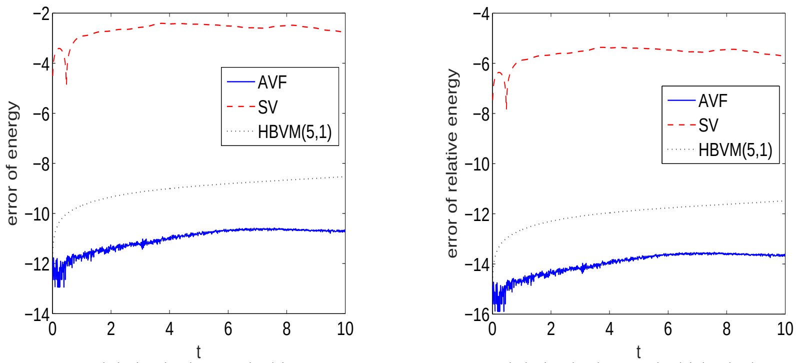


FIGURE 6. Circular of two ring solitons: contours of $\sin(u/2)$ for the numerical solutions at times $t = 0, 2, 4, 6, 8, 10$.



(a) $|E(t_n) - E(t_0)|$

(b) $|E(t_n) - E(t_0)|/E(t_0)$

FIGURE 7. The logarithms of the discrete energy error (a) and the relative discrete energy error (b).

for the two-dimensional Hamiltonian wave equations. Three illustrative numerical experiments were implemented and the numerical results show the convergence order of the spatial semidiscretisation and the remarkable conservative behaviour of the novel energy-conservation algorithm proposed in this paper.

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