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LAGRANGIAN APPROACH TO DERIVING ENERGY-PRESERVING NUMERICAL SCHEMES FOR THE EULER–LAGRANGE PARTIAL DIFFERENTIAL EQUATIONS *

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Abstract. We propose a Lagrangian approach to deriving energy-preserving finite difference schemes for the Euler–Lagrange partial differential equations. Noether's theorem states that the symmetry of time translation of Lagrangians yields the energy conservation law. We introduce a unique viewpoint on this theorem: "the symmetry of time translation of Lagrangians derives the Euler–Lagrange equation and the energy conservation law, simultaneously." The proposed method is a combination of a discrete counter part of this statement and the discrete gradient method. It is also shown that the symmetry of space translation derives momentum-preserving schemes. Finally, we discuss the existence of discrete local conservation laws.

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1. Introduction

In this paper, we propose a Lagrangian approach to deriving energy-preserving finite difference schemes for the Euler–Lagrange partial differential equations. Our approach is based on a combination of the symmetry of time translation of discrete Lagrangians and the discrete gradient method.

For PDEs that enjoy a conservation property, numerical schemes that inherit this property are often advantageous, in that the schemes are fairly stable, and yield qualitatively better numerical solutions in practice. Among such properties, the energy conservation law and symplecticity have received significant attention. However, the Zhong–Marsden theorem [71] and the stronger result for B-series methods by Chartier–Faou–Murua [15] show that an integrator cannot be both energy-preserving and symplectic[2]. Hence, methods on this subject are mainly divided into the corresponding two groups. See, for example, [8,21,33,65] for other structure-preserving methods. In this paper, energy-preserving schemes are of interest.

Keywords and phrases. Discrete gradient method, energy-preserving integrator, finite difference method, Lagrangian mechanics.

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[2]Precisely, the Zhong–Marsden theorem holds only for Hamiltonian ODEs. To date, a similar result for PDEs has not been obtained.

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Among energy-preserving schemes, application of the discrete gradient method to the Hamiltonian PDEs is highly successful ([13, 29, 39–41, 57, 63], and references therein). Alternatively, Furihata and Matsuo have developed the so-called "discrete variational derivative method", which is a kind of the discrete gradient method specialized for PDEs ([23–27,52–54,56], and references therein). Another way to obtain energy-preserving methods is to apply the projection method ([2,3,17,20,30,31,61,62,66,67], and references therein); however, in many cases, the discrete-gradient-type methods result in qualitatively better solutions.

The discrete-gradient-type methods typically use the Hamiltonian form of equations. These methods have been mainly developed for ODEs represented in the Hamiltonian form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = J(u)\nabla_u H,$$

where $H(u)$ is a Hamiltonian and $J(u)$ is a skew operator. This equation has the energy conservation law

$$\frac{\mathrm{d}H}{\mathrm{d}t} = 0.$$

$\bar{\nabla}H(u,v)$ is said to be a discrete gradient of H if $\bar{\nabla}H(u,v)$ satisfies

$$H(u) - H(v) = \bar{\nabla}H(u,v)\cdot(u-v), \quad \bar{\nabla}H(u,u) = \nabla H(u). \tag{1.1}$$

Once a discrete gradient is obtained, an energy-preserving numerical scheme is obtained by

$$\frac{U^{(n+1)} - U^{(n)}}{\Delta t} = \tilde{J}\bar{\nabla}H(U^{(n+1)}, U^{(n)})$$

where $U^{(n)}$ is an approximation of $u(n\Delta t)$ and $\tilde{J}$ is a skew operator that approximates $J(u)$. Because this scheme typically becomes a system of nonlinear equations, the Newton method is needed. It is straightforward to show that this scheme maintains the energy conservation property

$$\frac{H(U^{(n+1)}) - H(U^{(n)})}{\Delta t} = 0.$$

Because the scheme is defined in the same form as the Hamiltonian form of the equation, we say that this method is based on Hamiltonian mechanics. Thus, the following question naturally arises: *"Is it possible to construct energy-preserving schemes by using the discrete gradient method based on Lagrangian mechanics?"*

A natural way to discretize the Euler–Lagrange equation is the application of the principle of least action in discretized spaces. This approach yields excellent symplectic methods and is widely known as the variational integrator or discrete mechanics [12,22,37,44,49,50,68,69]. In particular, it is shown that if a carefully designed adaptive-time-stepping method is applied, a symplectic and energy-preserving method can be constructed [37]. On the other hand, to the best of our knowledge, no unified method exists that uses the discrete gradient method for deriving energy-preserving schemes based on Lagrangian mechanics. The aim of this paper is to develop such an approach.

Perhaps the main difficulty in developing a Lagrangian approach that derives energy-preserving methods is finding a natural definition of the discrete energy function. In classical field theory, the energy density functional is defined by

$$\mathcal{L} - u_t\frac{\partial \mathcal{L}}{\partial u_t}, \tag{1.2}$$

where $\mathcal{L}$ is a Lagrangian density to be considered. However, there are infinitely many ways to discretize u_t in (1.2), and there is no indication which one is the most appropriate.

Our approach is based on an observation on Noether's theorem. As is well-known, Noether's theorem states that symmetries derive conserved quantities. For example, the conservation of energy is derived from the symmetry of time translation. Similarly, the conservation of momentum is derived from the symmetry of space translation. In this paper, we introduce another viewpoint on this theorem: *if a Lagrangian has the symmetry of time translation, variation with respect to this symmetry derives the Euler–Lagrange equation and the energy conservation law, simultaneously*. Our method is a discrete counterpart of this statement. Because this statement can be easily derived from the standard proofs of the Noether theorem, our main contribution is to construct a discrete counter part of this statement and combine it with the discrete gradient method. In our method, we first discretize the Lagrangian density; then, we define the scheme as an approximation of the Euler–Lagrange equation that is obtained by evaluation of a difference of action sums with respect to the action of the generator of the discrete group corresponding to a given symmetry. Schemes derived by using this methodology automatically inherit the conservation property corresponding to the symmetry used. Thereby, in addition to deriving energy-preserving schemes, our method also derives other conservative schemes. We are still developing a general framework for other symmetries; however, we illustrate the idea by deriving momentum-preserving schemes from the spatial symmetry. In addition, because the Noether theorem also ensures the existence of a local conservation law [60], our schemes have a discrete analogue of this law.

However, our method ensures the conservation of only the chosen conserved quantity and nothing can be said on the behaviors of other quantities. Although the numerical test in Section 6 shows that the energy-preserving scheme for the nonlinear Klein–Gordon equation preserves the discrete momentum and the discrete angular momentum well, this may not be the case for other equations and other choices of discrete Lagrangian densities. Hence, the symmetry and conservation law that must be conserved should be carefully selected.

Although the author believes that the above procedure is first pointed out in this paper, several previous studies have examined relations between symmetries and conservation laws of difference equations in terms of the discrete Noether theorems. For example, Dorodnitsyn investigated relations between conservation laws and Lie point symmetries of difference equations [18,19]. Mansfield *et al.* introduced a discrete variational complex on lattices to find conservation laws [35,47]. Logan showed the discrete Noether theorem for the discrete Euler–Lagrange equations [46]. Energy behaviors of symplectic methods for the Maxwell equation are investigated by using the Noether theorem in Saitoh [64]. Symmetry also plays a very important role in the work on r-adaptive moving-mesh methods by Budd and Williams ([4–7,9–11,34], and references therein). We believe that there are at least two major differences between our approach and the other works:

- we use discrete symmetries, while continuous symmetries are usually adopted in the others, and
- we use the discrete gradient method.

However, there would be some relations between our method and these works, which should be investigated in future work.

From a practical point of view, it would be noteworthy that our approach naturally derives explicit or linearly implicit schemes in most cases, while, although some techniques for obtaining linearly implicit schemes have recently been developed [16,55], the usual application of the discrete gradient method to the Hamiltonian form yields nonlinearly implicit schemes. This is a desirable feature because it can dramatically reduce computational costs.

This paper is organized as follows.

- In Section 2, we provide a brief description of our approach. First, we recall the relation between the definition of the energy function in Lagrangian mechanics and Noether's theorem. Then we also recall how the energy-conservation law is obtained from the symmetry of time translation. This observation makes it possible to say that the symmetry of Lagrangians derives not only the conservation law, but also the Euler–Lagrange equation, at least formally.
- In Section 3, we introduce the notation used in this paper.
- In Section 4, we explain our unified approach to deriving energy-preserving finite difference schemes in detail.

- In Section 5, the use of spatial symmetry to derive momentum-preserving schemes is demonstrated. Although the general framework is not completely developed in this paper, we believe that the same procedure can be applied with almost arbitrary symmetries in principle.
- In Section 6, as an example, we derive an energy-preserving scheme and a momentum-preserving scheme for the nonlinear Klein–Gordon equation. In addition, we perform a numerical test in which these schemes are compared with the Marsden–Patrick–Shkoller scheme.
- In Section 7, a local theory of the proposed approach is presented. It is shown that our schemes also satisfy a (spatially) local conservation law. This implies that by using appropriate interpolation algorithms, it may be possible to use different time step sizes on each node. This result may be useful to overcome the constraint on step sizes due to the CFL condition.

2. Noether's theorem and key idea of proposed approach

In this paper, we propose a Lagrangian approach to deriving energy-preserving numerical schemes. The governing equation of Lagrangian mechanics is the Euler–Lagrange equation. In infinite dimensional cases, this equation is the Euler–Lagrange partial differential equation

$$\frac{\partial \mathcal{L}}{\partial u} - D_x \frac{\partial \mathcal{L}}{\partial u_x} - D_t \frac{\partial \mathcal{L}}{\partial u_t} = 0, \tag{2.1}$$

where $\mathcal{L}$ is a Lagrangian density, and D_x and D_y are the total derivatives [60]. For simplicity, we consider this equation on a one-dimensional interval $[0, L]$; however, our approach can be applied to multi-dimensional problems defined on complicated domains with nonuniform meshes in a straightforward manner. The energy and the momentum of this equation are defined as

$$\int_0^L \left(u_t \frac{\partial \mathcal{L}}{\partial u_t} - \mathcal{L} \right) \mathrm{d}x \tag{2.2}$$

and

$$\int_0^L \left(-u_x \frac{\partial \mathcal{L}}{\partial u_t} \right) \mathrm{d}x, \tag{2.3}$$

respectively (*e.g.* [1, 28, 42]).

Because we want to take a Lagrangian approach, we should start with giving a discrete Lagrangian density, and this requires a natural definition of discrete energy for the given discrete Lagrangian density. For example, because the energy function in Lagrangian mechanics (2.2) contains the term $u_t \partial \mathcal{L}/\partial u_t$, we need to discretize u_t to define a discrete energy function. However, because u_t can be discretized in infinitely many ways, it is not obvious which discretization is the natural choice regarding the given discrete Lagrangian.

To naturally introduce discrete energy, first we must recall how this conserved quantity was introduced as "energy" in classical mechanics. In the classical great textbooks, such as Landau–Lifshitz [42] and Goldstein–Poole–Safko [28], energy is defined as the conserved quantity that results from time homogeneity. For example, in Landau–Lifshitz [42], the following is noted:

> *"Not all integrals of the motion, however, are of equal importance in mechanics. There are some whose constancy is of profound significance, deriving from the fundamental homogeneity and isotropy of space and time".*

Next, by using the symmetry of time translation, a quantity, which is an ODE version of (2.2), is shown to be a first integral. Energy is introduced as this quantity. In addition, momentum is introduced by using the symmetry of space translation in the same way.

From this viewpoint, it seems natural to define discrete energy by symmetry, or equivalently by the Noether theorem. Next, we confirm how the energy conservation law stems from the symmetry of time translation of

Lagrangians. We show this in an elementary manner, because our method is a discrete analogue of it. Indeed, the following calculation fortunately suggests not only a natural definition of discrete energy, but also a method to derive a numerical scheme that preserves it.

Let g be the action of the one parameter group

$$g : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{R}^3, \quad (\delta t, (x, t, u)) \mapsto (x, t + \delta t, u),$$

and suppose that a Lagrangian $\mathcal{L}$ has the symmetry with respect to this action, *i.e.*, $\mathcal{L}$ is independent of t. More precisely, the prolongation of u with respect to the action g is

$$\tilde{u}(\tilde{t}, \tilde{x}) = u(\tilde{t} - \delta t, x), \quad \tilde{t} = t + \delta t, \quad \tilde{x} = x,$$

and the symmetry implies that the difference of the action integrals must vanish:

$$0 = \int_0^T \int_0^L \mathcal{L}(\tilde{x}, \tilde{t}, \tilde{u}, \tilde{u}_{\tilde{x}}, \tilde{u}_{\tilde{t}}) \mathrm{d}\tilde{t} - \int_0^T \int_0^L \mathcal{L}(x, t, u, u_x, u_t) \mathrm{d}t.$$

The right hand side is rewritten as

$$= \int_0^T \int_0^L \mathcal{L}(x, t + \delta t, u, u_x, u_t) \mathrm{d}t - \int_0^T \int_0^L \mathcal{L}(x, t, u, u_x, u_t) \mathrm{d}t \tag{2.4}$$

$$= \int_{\delta t}^{T+\delta t} \int_0^L \mathcal{L}(x, t, u(t - \delta t, x), u_x(t - \delta t, x), u_t(t - \delta t, x)) \mathrm{d}t - \int_0^T \int_0^L \mathcal{L}(x, t, u, u_x, u_t) \mathrm{d}t. \tag{2.5}$$

In the following, we often start with this expression to avoid repetition of the above calculation. Multiplication of $1/\delta t$ to (2.5) gives

$$\begin{aligned} 0 = {} & \frac{1}{\delta t} \int_T^{T+\delta t} \int_0^L \mathcal{L}\left(x, t, u(t - \delta t, x), u_x(t - \delta t, x), u_t(t - \delta t, x)\right) \mathrm{d}x\mathrm{d}t - \frac{1}{\delta t} \int_0^{\delta t} \int_0^L \mathcal{L}\left(x, t, u, u_x, u_t\right) \mathrm{d}x\mathrm{d}t \\ & + \frac{1}{\delta t} \int_{\delta t}^T \int_0^L \left(\mathcal{L}\left(x, t, u(t - \delta t, x), u_x(t - \delta t, x), u_t(t - \delta t, x)\right) - \mathcal{L}\left(x, t, u, u_x, u_t\right)\right) \mathrm{d}x\mathrm{d}t. \end{aligned}$$

Under the assumption, for simplicity, of the periodic boundary condition, letting $\delta t \to 0$ gives

$$\begin{aligned} & \to \int_0^L \mathcal{L}\mathrm{d}x \mid_{t=T} - \int_0^L \mathcal{L}\mathrm{d}x \mid_{t=0} - \int_0^T \int_0^L \left(\frac{\partial \mathcal{L}}{\partial u} u_t + \frac{\partial \mathcal{L}}{\partial u_x} u_{xt} + \frac{\partial \mathcal{L}}{\partial u_t} u_{tt}\right) \mathrm{d}x\mathrm{d}t \\ & = - \int_0^T \int_0^L u_t \left(\frac{\partial \mathcal{L}}{\partial u} - D_x \frac{\partial \mathcal{L}}{\partial u_x} - D_t \frac{\partial \mathcal{L}}{\partial u_t}\right) \mathrm{d}x\mathrm{d}t \qquad (2.6) \\ & \quad + \int_0^L \left(\mathcal{L} - u_t \frac{\partial \mathcal{L}}{\partial u_t}\right) \mathrm{d}x \mid_{t=T} - \int_0^L \left(\mathcal{L} - u_t \frac{\partial \mathcal{L}}{\partial u_t}\right) \mathrm{d}x \mid_{t=0} . \qquad (2.7) \end{aligned}$$

Because the equation is defined by the Euler–Lagrange equation (2.1), it follows that

$$\int_0^L \left(\mathcal{L} - u_t \frac{\partial \mathcal{L}}{\partial u_t}\right) \mathrm{d}x \mid_{t=T} - \int_0^L \left(\mathcal{L} - u_t \frac{\partial \mathcal{L}}{\partial u_t}\right) \mathrm{d}x \mid_{t=0} = 0,$$

which shows the energy conservation law.

Our approach is based on the following observation. Although we have described the above calculation as an elementary proof of Noether's theorem, if we pay close attention to (2.6) and (2.7), it is possible to say that "the symmetry of time translation of Lagrangians derives the Euler–Lagrange equation and the conserved quantity, *i.e.*, the energy function, simultaneously." Therefore if we can perform a similar calculation after discretization, we will obtain at once a natural definition of discrete energy and a discrete analogue of the Euler–Lagrange equation that preserves this discrete energy. After introducing some definitions and notation in Section 3, we will show the feasibility of this idea in Section 4.

Remark 2.1. The idea presented above can be applied with respect to other symmetries. For example, a similar calculation with spatial symmetry yields

$$-\int_0^T\int_0^L u_x\left(\frac{\partial\mathcal{L}}{\partial u}-D_x\frac{\partial\mathcal{L}}{\partial u_x}-D_y\frac{\partial\mathcal{L}}{\partial u_t}\right)\mathrm{d}x\mathrm{d}t \tag{2.8}$$

$$+\int_0^L\left(-u_x\frac{\partial\mathcal{L}}{\partial u_t}\right)\mathrm{d}x\mid_{t=T}-\int_0^L\left(-u_x\frac{\partial\mathcal{L}}{\partial u_t}\right)\mathrm{d}x\mid_{t=0}=0, \tag{2.9}$$

which shows the momentum conservation property. In Section 5, we show that momentum-preserving schemes can be derived from spatial symmetries with the same approach presented in Section 4.

Remark 2.2. From a technical point of view, we used the chain rule and the integration-by-parts formula to obtain (2.6) and (2.7). Therefore, to realize our idea presented above, discrete versions of these formulas are required. Fortunately, such formulas exist. Specifically, we can use the discrete gradient method as a discrete version of the chain rule and the summation-by-parts formula as that of the integration-by-parts formula. These techniques are summarized in Section 3. In addition, the discrete gradient method is used as the discrete version of the chain rule when this method is applied in the standard manner to the Hamiltonian form of equations.

Remark 2.3. It is not our intention to provide an alternative approach of discrete "mechanics." The aim of this study is to develop an alternative "technique" to deriving energy-preserving numerical schemes by using the discrete gradient method. Indeed the above idea is not admissible as a principle of mechanics. It simply means that "the symmetry of time translation of Lagrangians *formally* derives the Euler–Lagrange equation and the conserved quantity."

3. Notation and definitions

In this section, we summarize the notation and definitions used in this paper.

We discretize space and time by the standard uniform grids with step sizes Δx and Δt. We denote by $U_j^{(n)}$ an approximated value of $u(n\Delta t, j\Delta x)$. The finite difference operators that approximate the partial differential operators are denoted by

$$\delta_t^+U_j^{(n)}=\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t},\quad \delta_t^-U_j^{(n)}=\frac{U_j^{(n)}-U_j^{(n-1)}}{\Delta t},\quad \delta_t^{\langle1\rangle}U_j^{(n)}=\frac{U_j^{(n+1)}-U_j^{(n-1)}}{2\Delta t},$$
$$\delta_x^+U_j^{(n)}=\frac{U_{j+1}^{(n)}-U_j^{(n)}}{\Delta x},\quad \delta_x^-U_j^{(n)}=\frac{U_j^{(n)}-U_{j-1}^{(n)}}{\Delta x},\quad \delta_x^{\langle1\rangle}U_j^{(n)}=\frac{U_{j+1}^{(n)}-U_{j-1}^{(n)}}{2\Delta x},$$
$$\delta_t^{\langle2\rangle}U_j^{(n)}=\frac{U_j^{(n+1)}-2U_j^{(n)}+U_j^{(n-1)}}{(\Delta t)^2},\quad \delta_x^{\langle2\rangle}U_j^{(n)}=\frac{U_{j+1}^{(n)}-2U_j^{(n)}+U_{j-1}^{(n)}}{(\Delta x)^2}.$$

Corresponding to these operators, the summation-by-parts formulas

$$\Delta x\sum_{j=1}^M U_j^{(n)}\left(\delta_x^+V_j^{(n)}\right)+\Delta x\sum_{j=1}^M V_j^{(n)}\left(\delta_x^-U_j^{(n)}\right)=U_M^{(n)}V_{M+1}^{(n)}-U_0^{(n)}V_1^{(n)}, \tag{3.1}$$

$$\Delta t\sum_{n=1}^N U_j^{(n)}\left(\delta_t^+V_j^{(n)}\right)+\Delta t\sum_{n=1}^N V_j^{(n)}\left(\delta_t^-U_j^{(n)}\right)=U_j^{(N)}V_j^{(N+1)}-U_j^{(0)}V_j^{(1)} \tag{3.2}$$

hold.

Remark 3.1. For simplicity, in this paper, we use only these difference operators; however, other difference operators with higher-order accuracy can be used. The summation-by-parts formula for general difference operators is available in [46, 59, 70].

Next, to simplify notation, we define the discrete 1st prolongation of $U_j^{(n)}$ by

$$\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)} := (U_j^{(n)}, \delta_x^+ U_j^{(n)}, \delta_x^- U_j^{(n)}, \delta_t^+ U_j^{(n)}, \delta_t^- U_j^{(n)}).$$

We call a functional $\mathcal{L}_{\mathrm{d}}$ of a 7-tuple $(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})$ to $\mathbb{R}$ a discrete Lagrangian density and the sum

$$\mathcal{S}_{\mathrm{d}} := \sum_{n=1}^{N}\sum_{j=1}^{M} \mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\Delta x \Delta t$$

the action sum. These definitions are essentially same as those in discrete mechanics [50, 68].

In our method, discrete gradients of discrete Lagrangian densities play an important role, because, as is shown in (1.1), these provide a discrete analogue of the chain rule that is used to calculate the variation of action sums. In this paper, discrete gradients of a discrete Lagrangian density are denoted by

$$\bar{\nabla}\mathcal{L}_{\mathrm{d}}(j, n, V, U) = \left(\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (V,U)}\right), \left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (V,U)_{x,+}}\right), \left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (V,U)_{x,-}}\right), \left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (V,U)_{t,+}}\right), \left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (V,U)_{t,-}}\right)\right)^{\top}. \tag{3.3}$$

These terms can be arbitrarily chosen as long as the discrete chain rule

$$\mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)}V_j^{(n)}) - \mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) = \bar{\nabla}\mathcal{L}_{\mathrm{d}} \cdot \left(\mathrm{pr}_{\mathrm{d}}^{(1)}(V_j^{(n)} - U_j^{(n)})\right)^{\top}$$

holds. A discrete gradient can be obtained in various ways, such as the coordinate increment method [36], the Furihata method [23] and the average vector field (AVF) method [13, 57, 63]. For example, the discrete gradient by the AVF method is given by

$$\bar{\nabla}\mathcal{L}_{\mathrm{d}}(j, n, V, U) = \int_0^1 (\nabla \mathcal{L}_{\mathrm{d}})(j, n, \xi(\mathrm{pr}_{\mathrm{d}}^{(1)}V) + (1-\xi)(\mathrm{pr}_{\mathrm{d}}^{(1)}U))\mathrm{d}\xi,$$

where

$$\nabla \mathcal{L}_{\mathrm{d}} = \left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial U}, \frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (\delta_x^+ U)}, \frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (\delta_x^- U)}, \frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (\delta_t^+ U)}, \frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial (\delta_t^- U)}\right)^{\top}.$$

In most cases, this method gives the same discrete gradient as that by the Furihata method. In addition, it is shown in [14] that the AVF method for Hamiltonian ODEs is conjugate-symplectic of order 4.

4. Lagrangian approach to deriving energy-preserving schemes by using the discrete gradient method

Let g_{d} be the action of the infinite cyclic group

$$g_{\mathrm{d}} : \mathbb{Z} \times (\mathbb{Z}^2 \times \mathbb{R}) \to (\mathbb{Z}^2 \times \mathbb{R}), \quad (z, (j, n, U)) \mapsto (j, n - z, U),$$

and suppose that the given discrete Lagrangian density $\mathcal{L}_{\mathrm{d}}$ has the symmetry with respect to this action, that is,

$$\mathcal{L}_{\mathrm{d}}(j, n - z, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) = \mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})$$

for any $z \in \mathbb{Z}$. Then, the difference of the action sums yields

$$\frac{1}{\Delta t}\left(\sum_{n=1}^{N}\sum_{j=1}^{M} \mathcal{L}_{\mathrm{d}}(j, n+1, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\Delta x \Delta t - \sum_{n=1}^{N}\sum_{j=1}^{M} \mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\Delta x \Delta t\right) = 0,$$

which is a discrete counter part of (2.4). Rearranging this summation, we obtain a discrete analogue of (2.5)

$$0 = \frac{1}{\Delta t}\left(\sum_{n=2}^{N+1}\sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n-1)})\Delta x\Delta t - \sum_{n=1}^{N}\sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\Delta x\Delta t\right)$$

and

$$\begin{aligned}
&= \frac{1}{\Delta t}\left(\sum_{n=2}^{N}\sum_{j=1}^{M}\left(\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n-1)}) - \mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\right)\right)\Delta x\Delta t\\
&\quad + \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,N+1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(N)})\Delta x - \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(1)})\Delta x\\
&= \frac{1}{\Delta t}\left(\sum_{n=2}^{N}\sum_{j=1}^{M}\left(\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n-1)}) - \mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\right)\right)\Delta x\Delta t\\
&\quad + \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,N,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(N)})\Delta x - \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(1)})\Delta x.
\end{aligned}$$

By using the discrete gradient method (3.3), we obtain

$$\begin{aligned}
&= \frac{1}{\Delta t}\sum_{n=2}^{N}\sum_{j=1}^{M}\bar{\nabla}\mathcal{L}_{\mathrm{d}}\cdot\left(\mathrm{pr}_{\mathrm{d}}^{(1)}(U_j^{(n-1)} - U_j^{(n)})\right)^{\top}\Delta x\Delta t + \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,N,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(N)})\Delta x - \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(1)})\Delta x\\
&= -\sum_{n=2}^{N}\sum_{j=1}^{M}\left\{\delta_t^- U_j^{(n)}\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})}\right) + \delta_t^-\delta_x^+ U_j^{(n)}\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{x,+}}\right)\right.\\
&\quad + \delta_t^-\delta_x^- U_j^{(n)}\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{x,-}}\right) + \delta_t^-\delta_t^+ U_j^{(n)}\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,+}}\right)\\
&\quad \left. + \delta_t^-\delta_t^- U_j^{(n)}\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,-}}\right)\right\}\Delta x\Delta t + \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,N,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(N)})\Delta x - \sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j,1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(1)})\Delta x.
\end{aligned}$$

Applying the summation-by-parts formula (3.1) and (3.2), we have

$$\begin{aligned}
&= -\sum_{n=2}^{N}\sum_{j=1}^{M}\left(\delta_t^- U_j^{(n)}\right)\left\{\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})}\right) - \delta_x^-\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{x,+}}\right)\right.\\
&\quad \left. - \delta_x^+\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{x,-}}\right) - \delta_t^-\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,+}}\right) - \delta_t^+\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,-}}\right)\right\}\Delta x\Delta t\\
&\quad - \sum_{n=2}^{N}\left(\left(\delta_t^- U_{M+1}^{(n)}\right)\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_M^{(n-1)},U_M^{(n)})_{x,+}}\right) - \left(\delta_t^- U_1^{(n)}\right)\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_0^{(n-1)},U_0^{(n)})_{x,+}}\right)\right)\Delta t\\
&\quad - \sum_{n=2}^{N}\left(\left(\delta_t^- U_M^{(n)}\right)\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_{M+1}^{(n-1)},U_{M+1}^{(n)})_{x,-}}\right) - \left(\delta_t^- U_0^{(n)}\right)\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_1^{(n-1)},U_1^{(n)})_{x,-}}\right)\right)\Delta t\\
&\quad - \sum_{j=1}^{M}\left(\left(\delta_t^- U_j^{(N+1)}\right)\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(N-1)},U_j^{(N)})_{t,+}}\right) - \left(\delta_t^- U_j^{(2)}\right)\left(\frac{\partial\mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(0)},U_j^{(1)})_{t,+}}\right)\right)\Delta x
\end{aligned}$$

$$-\sum_{j=1}^{M}\left(\left(\delta_t^- U_j^{(N)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(N)}, U_j^{(N+1)})_{t,-}}\right)-\left(\delta_t^- U_j^{(1)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(1)}, U_j^{(2)})_{t,-}}\right)\right)\Delta x$$
$$+\sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j, N, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(N)})\Delta x-\sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j, 1, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(1)})\Delta x.$$

Therefore, if we define a scheme by the following discrete analogue of the Euler–Lagrange equation

$$\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)}, U_j^{(n)})}\right)-\delta_x^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)}, U_j^{(n)})_{x,+}}\right)-\delta_x^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)}, U_j^{(n)})_{x,-}}\right)$$
$$-\delta_t^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)}, U_j^{(n)})_{t,+}}\right)-\delta_t^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)}, U_j^{(n)})_{t,-}}\right)=0, \tag{4.1}$$

we obtain the following discrete energy conservation law.

Theorem 4.1. *Suppose that $U_j^{(n)}$ is a numerical solution of the scheme (4.1) under a boundary condition that satisfies*

$$\left(\delta_t^- U_{M+1}^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_M^{(n-1)}, U_M^{(n)})_{x,+}}\right)+\left(\delta_t^- U_M^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{M+1}^{(n-1)}, U_{M+1}^{(n)})_{x,-}}\right)$$
$$-\left(\delta_t^- U_1^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_0^{(n-1)}, U_0^{(n)})_{x,+}}\right)-\left(\delta_t^- U_0^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_1^{(n-1)}, U_1^{(n)})_{x,-}}\right)=0.$$

Then, the following discrete energy conservation law holds:

$$\sum_{j=1}^{M}\mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(n)})\Delta x-\sum_{j=1}^{M}\left(\left(\delta_t^- U_j^{(n+1)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)}, U_j^{(n)})_{t,+}}\right)\right.$$
$$\left.+\left(\delta_t^- U_j^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)}, U_j^{(n+1)})_{t,-}}\right)\right)\Delta x=\mathrm{const}.$$

Definition 4.2. We call the discrete analogue (4.1) of the Euler–Lagrange equation *the (g_{d}, $\bar{\nabla}$)-discrete Euler–Lagrange equation*.

Remark 4.3. There exist some other discrete analogues of the Euler–Lagrange equation. For example, the most famous one would be the one in discrete mechanics [50, 68], which is called *the discrete Euler–Lagrange equation*. We call the one in our approach the (g_{d}, $\bar{\nabla}$)-discrete Euler–Lagrange equation in order to distinguish it from the others.

Remark 4.4. A major difference between our approach and other studies related to the discrete Noether theorem is that we use a discrete symmetry to derive numerical schemes, while the others adopt continuous symmetries. Another difference is that we use the discrete gradient method.

Remark 4.5. Our theory ensures the conservation of only one chosen conserved quantity while the other conserved quantities may or may not be conserved. Indeed, although the AVF method is conjugate-symplectic of order 4 for Hamiltonian ODEs, this is not necessarily true for this Lagrangian method. Practically, the numerical test in Section 6 shows that the energy-preserving scheme for the nonlinear Klein–Gordon equation preserves the discrete momentum and the discrete angular momentum well; however, this may not be the case for other equations.

Remark 4.6. The order of accuracy of the schemes is determined as follows:

- the spatial order of accuracy is determined by the accuracy of the discrete Lagrangian density,
- the temporal order of accuracy is determined by the accuracies of the discrete Lagrangian density and the discrete gradient.

In this paper, for simplicity, we have used the forward and backward difference operators; nevertheless, other difference operators, such as those of higher-order accuracy and the pseudo-spectral difference operator, can be used. The summation-by-parts formulas corresponding to general difference operators are available in [46,59,70]. Therefore, high order schemes in the spatial direction are obtained in a straightforward manner. About the temporal direction, there exist a few results on the discrete gradient of higher order accuracy. One such example is a high-order generalization of the Gonzalez discrete gradient by Matsuo [27, 51]. This method could be combined with our method. Another choice could be the collocation method by Hairer [32], which is a higher-order extension of the AVF method. This method has a conjugate-symplecticity of higher order if the method is applied to Hamiltonian ODEs.

Remark 4.7. We assume that the spatial indices belong to entire $\mathbb{Z}$. This implies that we also assume that boundary conditions are imposed by the so-called ghost cell method [43]. In this method, the computational domain is extended to include additional nodes, which are called ghost nodes or ghost cells, outside the boundaries. The boundary condition is imposed by appropriately setting the values on these nodes. For example, the periodic boundary condition is imposed by setting $U_{-1}^{(n)} = U_{M-1}^{(n)}, U_0^{(n)} = U_M^{(n)}, U_{M+1}^{(n)} = U_1^{(n)}, U_{M+2}^{(n)} = U_2^{(n)}$, etc. As another example, the Neumann boundary condition $u_x = 0$ can be discretized into $\delta_x^{\langle 1\rangle} U_0^{(n)} = 0$, which implies $U_{-1}^{(n)} = U_1^{(n)}$. For more complicated boundary conditions, see [43] and references therein.

5. Symmetry of space translation and momentum-preserving schemes

In this section, we discuss the use of other symmetries. We believe that general divergence symmetries [60] can be applied in our approach; however, we have not been successful in obtaining a suitable definition of "discrete divergence symmetry." Thus, we illustrate the idea by deriving momentum-preserving schemes from spatial symmetry.

The schemes are obtained in exactly the same way as in the previous section. Suppose that a discrete Lagrangian density has a symmetry with respect to the action of the infinite cyclic group h_{d}

$$h_{\mathrm{d}} : \mathbb{Z} \times (\mathbb{Z}^2 \times \mathbb{R}) \to (\mathbb{Z}^2 \times \mathbb{R}), \quad (z, (j, n, U)) \mapsto (j - z, n, U),$$

that is,

$$\mathcal{L}_{\mathrm{d}}(j - z, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(n)}) = \mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(n)}).$$

Then, the difference of the action sums with respect to this symmetry yields

$$\frac{1}{\Delta x}\left(\sum_{n=1}^{N}\sum_{j=0}^{M} \mathcal{L}_{\mathrm{d}}(j+1, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(n)})\Delta x \Delta t - \sum_{n=1}^{N}\sum_{j=0}^{M} \mathcal{L}_{\mathrm{d}}(j, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_j^{(n)})\Delta x \Delta t\right) = 0.$$

By performing the same calculations as in the energy-preserving schemes, we obtain

$$
\begin{aligned}
0 = &-\sum_{n=1}^{N}\sum_{j=1}^{M}\left(\delta_x^- U_j^{(n)}\right)\left\{\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})}\right) - \delta_x^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{x,+}}\right)\right.\\
&\left. - \delta_x^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{x,-}}\right) - \delta_t^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{t,+}}\right) - \delta_t^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{t,-}}\right)\right\}\Delta x\Delta t\\
&-\sum_{n=1}^{N}\left(\left(\delta_x^- U_{M+1}^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{M-1}^{(n)}, U_M^{(n)})_{x,+}}\right) - \left(\delta_x^- U_1^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{-1}^{(n)}, U_0^{(n)})_{x,+}}\right)\right)\Delta t\\
&-\sum_{n=1}^{N}\left(\left(\delta_x^- U_M^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_M^{(n)}, U_{M+1}^{(n)})_{x,-}}\right) - \left(\delta_x^- U_0^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_0^{(n)}, U_1^{(n)})_{x,-}}\right)\right)\Delta t\\
&-\sum_{j=1}^{M}\left(\left(\delta_x^- U_j^{(N+1)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(N)}, U_j^{(N)})_{t,+}}\right) - \left(\delta_x^- U_j^{(1)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(0)}, U_j^{(0)})_{t,+}}\right)\right)\Delta x\\
&-\sum_{j=1}^{M}\left(\left(\delta_x^- U_j^{(N)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(N+1)}, U_j^{(N+1)})_{t,-}}\right) - \left(\delta_x^- U_j^{(0)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(1)}, U_j^{(1)})_{t,-}}\right)\right)\Delta x\\
&+\sum_{n=1}^{N}\mathcal{L}_{\mathrm{d}}(M, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_M^{(n)})\Delta t - \sum_{n=1}^{N}\mathcal{L}_{\mathrm{d}}(0, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_0^{(n)})\Delta t.
\end{aligned}
$$

Thus, if we define the scheme by

$$
\begin{aligned}
&\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})}\right) - \delta_x^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{x,+}}\right) - \delta_x^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{x,-}}\right)\\
&- \delta_t^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{t,+}}\right) - \delta_t^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{t,-}}\right) = 0,
\end{aligned}
\tag{5.1}
$$

which we call the $(h_{\mathrm{d}}, \bar{\nabla})$-discrete Euler–Lagrange equation, we have the following discrete momentum conservation law:

Theorem 5.1. *Suppose that $U_j^{(n)}$ is a numerical solution of the scheme (5.1) under a boundary condition that satisfies*

$$
\begin{aligned}
&\mathcal{L}_{\mathrm{d}}(M, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_M^{(n)}) - \left(\delta_x^- U_{M+1}^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{M-1}^{(n)}, U_M^{(n)})_{x,+}}\right) - \left(\delta_x^- U_M^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_M^{(n)}, U_{M+1}^{(n)})_{x,-}}\right)\\
&= \mathcal{L}_{\mathrm{d}}(0, n, \mathrm{pr}_{\mathrm{d}}^{(1)} U_0^{(n)}) - \left(\delta_x^- U_1^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{-1}^{(n)}, U_0^{(n)})_{x,+}}\right) - \left(\delta_x^- U_0^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_0^{(n)}, U_1^{(n)})_{x,-}}\right).
\end{aligned}
$$

Then the following discrete momentum conservation law holds:

$$
\sum_{j=1}^{M}\left(\left(\delta_x^- U_j^{(n+1)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)}, U_j^{(n)})_{t,+}}\right) + \left(\delta_x^- U_j^{(n)}\right)\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n+1)}, U_j^{(n+1)})_{t,-}}\right)\right)\Delta x = \text{const.}
$$

6. Numerical example

In this section, we present an energy-preserving scheme and a momentum-preserving scheme for the nonlinear Klein–Gordon equation and perform a numerical comparison with the Marsden–Patrick–Shkoller scheme.

We derive an energy-preserving scheme for the nonlinear Klein–Gordon equation

$$u_{tt} - u_{xx} = \phi'(u),\ u(t, x + L) = u(t, x) \tag{6.1}$$

whose Lagrangian density is

$$\mathcal{L}(x, t, u, u_x, u_t) = -\frac{1}{2}u_t^2 + \frac{1}{2}u_x^2 - \phi(u). \tag{6.2}$$

The Lagrangian density of the nonlinear Klein–Gordon equation has the time and spatial symmetries, and hence the energy function

$$E(t) = \int_0^L \left(\frac{1}{2}u_t^2 + \frac{1}{2}u_x^2 - \phi(u)\right) \mathrm{d}x$$

and the momentum function

$$M(t) = \int_0^L u_x u_t \mathrm{d}x$$

are conserved.

We introduce a discrete Lagrangian density for this equation by

$$\mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) = -\frac{1}{4}\left((\delta_t^+ U_j^{(n)})^2 + (\delta_t^- U_j^{(n)})^2\right) + \frac{1}{4}\left((\delta_x^+ U_j^{(n)})^2 + (\delta_x^- U_j^{(n)})^2\right) - \phi(U_j^{(n)}).$$

This discrete Lagrangian has the symmetry of time translation

$$\mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) = \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}).$$

If the AVF method [57, 63], or equivalently the Furihata method [23], is employed as the discrete gradient, the procedure shown in Section 4 yields the following $(g_\mathrm{d}, \bar{\nabla})$-discrete Euler–Lagrange equation

$$\delta_t^- \delta_t^{\langle 1\rangle} U_j^{(n)} - \delta_x^{\langle 2\rangle}\left(\frac{U_j^{(n)} + U_j^{(n-1)}}{2}\right) - \int_0^1 \phi'(\xi U_j^{(n)} + (1-\xi)U_j^{(n-1)})\mathrm{d}\xi = 0. \tag{6.3}$$

This scheme has the following discrete energy conservation law

$$\sum_{j=1}^{M}\left((\delta_t^{\langle 1\rangle} U_j^{(n)})^2 + \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)})\right)\Delta x = \text{const.},$$

if the boundary condition satisfies

$$-\frac{1}{4}\left[(\delta_x^+(U_M^{(n)} + U_M^{(n-1)}))(\delta_t^-(U_{M+1}^{(n)} + U_M^{(n)}))\right] + \frac{1}{4}\left[(\delta_x^+(U_0^{(n)} + U_0^{(n-1)}))(\delta_t^-(U_1^{(n)} + U_0^{(n)}))\right] = 0.$$

Remark 6.1. This scheme is identical to the energy-preserving explicit scheme by Furihata [25]; however, the scheme in [25] is derived in a different manner.

Similarly, by using the spatial symmetry, we get the $(h_\mathrm{d}, \bar{\nabla})$-discrete Euler–Lagrange equation

$$\delta_t^{\langle 2\rangle}\left(\frac{U_{j-1}^{(n)} + U_j^{(n)}}{2}\right) - \delta_x^{\langle 2\rangle}\left(\frac{U_{j-1}^{(n)} + U_j^{(n)}}{2}\right) - \int_0^1 \phi'(\xi U_j^{(n)} + (1-\xi)U_{j-1}^{(n)})\mathrm{d}\xi = 0, \tag{6.4}$$

which satisfies the discrete momentum conservation law

$$\sum_{j=1}^{M} \frac{1}{4}\left[(\delta_x^- U_j^{(n+1)})\cdot(\delta_t^+(U_{j-1}^{(n)}+U_j^{(n)}))+(\delta_x^- U_j^{(n)})\cdot(\delta_t^+(U_{j-1}^{(n+1)}+U_j^{(n+1)}))\right]\Delta x=\text{const.},$$

if the boundary condition satisfies

$$\mathcal{L}_{\mathrm{d}}(M,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_M^{(n)})-(\delta_x^{\langle 1\rangle}U_M^{(n)})^2-\mathcal{L}_{\mathrm{d}}(1,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_1^{(n)})+(\delta_x^{\langle 1\rangle}U_1^{(n)})^2=0.$$

Next, we performed a numerical test to compare these two schemes with the Marsden–Patrick–Shkoller scheme [48]

$$\begin{aligned}&\frac{1}{2}\delta_t^{\langle 2\rangle}U_j^{(n)}+\frac{1}{4}\delta_t^{\langle 2\rangle}U_{j+1}^{(n)}+\frac{1}{4}\delta_t^{\langle 2\rangle}U_{j-1}^{(n)}-\delta_x^{\langle 2\rangle}U_j^{(n)}+\frac{1}{4}\left(\phi'(\bar{U}_j^{(n)})+\phi'(\bar{U}_{j-1}^{(n)})+\phi'(\bar{U}_j^{(n-1)})+\phi'(\bar{U}_{j-1}^{(n-1)})\right)=0,\\&\bar{U}_j^{(n)}=\frac{1}{4}\left(U_j^{(n)}+U_{j+1}^{(n)}+U_j^{(n+1)}+U_{j+1}^{(n+1)}\right).\end{aligned}\tag{6.5}$$

Because this scheme is a system of nonlinear equations, we used the Broyden method to solve it [38]. Motivated by the numerical test presented in [45], we solved the nonlinear Klein–Gordon equation under the periodic boundary condition

$$u_{tt}-u_{xx}=\phi'(u),\ \phi(u)=\frac{u^2}{2}-\frac{u^4}{4\pi^2},\ u(t,x+L)=u(t,x),\ L=100\tag{6.6}$$

with the initial condition

$$u(t,x)=\pi\left(\tanh\frac{x-48.5+\beta t}{\sqrt{2(1-\beta^2)}}+\tanh\frac{-(x-51.5)+\beta t}{\sqrt{2(1-\beta^2)}}-1\right)$$

for $t\le 0$. We set $\beta=0.2$. The numerical solutions obtained under these conditions are of breather-type. We set Δt to 0.1 and used a uniform grid consisting of 501 nodes.

The numerical solutions obtained by (6.3), (6.4) and (6.5) are shown in Figures 1– 3 respectively. We do not observe any significant differences between these figures. Next, we compared the behaviors of the conserved quantities. The evolutions of the energies, the momenta and the angular momenta are presented in Figures 4–6, respectively. The discrete angular momentum that we used is a linear combination of the discrete energy density and the discrete momentum density:

$$\begin{aligned}\sum_{j=1}^{M}\Bigg[&j\Delta x\left((\delta_t^{\langle 1\rangle}U_j^{(n)})^2+\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\right)\\&+\frac{n\Delta t}{4}\left[(\delta_x^- U_j^{(n+1)})\cdot(\delta_t^+(U_{j-1}^{(n)}+U_j^{(n)}))+(\delta_x^- U_j^{(n)})\cdot(\delta_t^+(U_{j-1}^{(n+1)}+U_j^{(n+1)}))\right]\Bigg]\Delta x.\end{aligned}$$

As shown in Figure 4, the discrete energy of the energy-preserving scheme is exactly conserved. In this case, the discrete energy is also well preserved by the momentum-preserving scheme and the Marsden–Patrick–Shkoller scheme. The results presented in Figure 5 are somewhat surprising. All schemes preserve the discrete momentum well. Actually, the Marsden–Patrick–Shkoller scheme performs the best, and surprisingly, the momentum-preserving scheme performs the worst. This behavior is caused by the rounding errors. In fact, when we performed the computation in quadruple-precision, the discrete momentum of the momentum-preserving scheme was preserved up to 10^{-31}. Conversely, the Marsden–Patrick–Shkoller scheme has the modified momentum conservation law that is guaranteed by the backward error analysis, and therefore is not much affected by the rounding errors. This is possibly why this scheme is "more conservative" than the momentum-preserving scheme. Although the

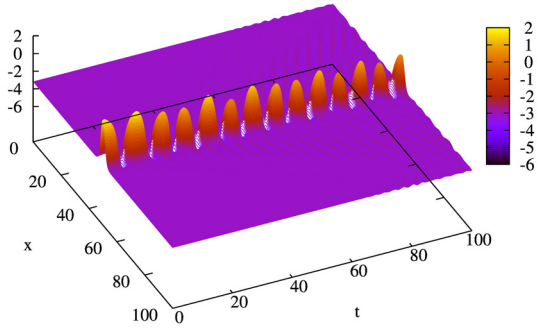

FIGURE 1. The numerical solution of the nonlinear Klein–Gordon equation (6.6) obtained by the energy-preserving scheme (6.3).

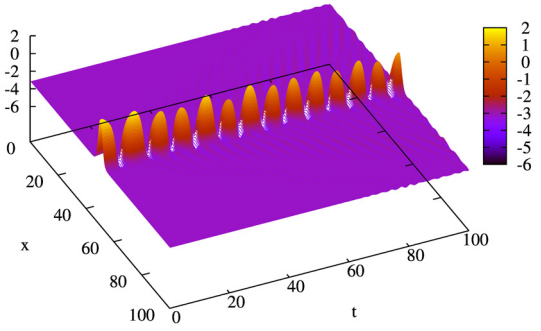

FIGURE 2. The numerical solution of the nonlinear Klein–Gordon equation (6.6) obtained by the momentum-preserving scheme (6.4).

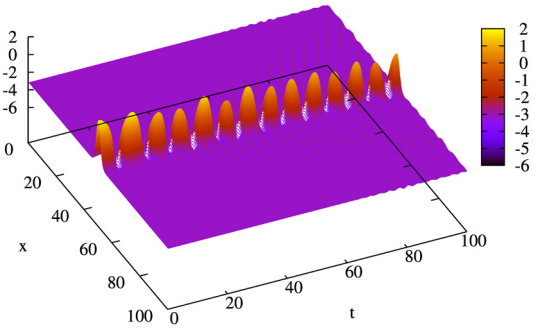

FIGURE 3. The numerical solution of the nonlinear Klein–Gordon equation (6.6) obtained by the Marsden–Patrick–Shkoller scheme (6.5).

momentum by the energy-preserving scheme is oscillatory, it exhibits small deviations. The behaviors of the discrete angular momenta are similar to those of the discrete energies; actually, the energy-preserving scheme preserves it very well. This may be due to the fact that in this case the angular momentum mostly consists of the energy.

In summary, although the discrete conservation property is proved only for energy or momentum, in the test case considered, these schemes also preserve other conserved quantities well; actually, their performance was not much worse than the Marsden–Patrick–Shkoller scheme. In particular, considering that the energy-preserving scheme is an explicit scheme, this scheme could be a method of choice. The good performance of our schemes

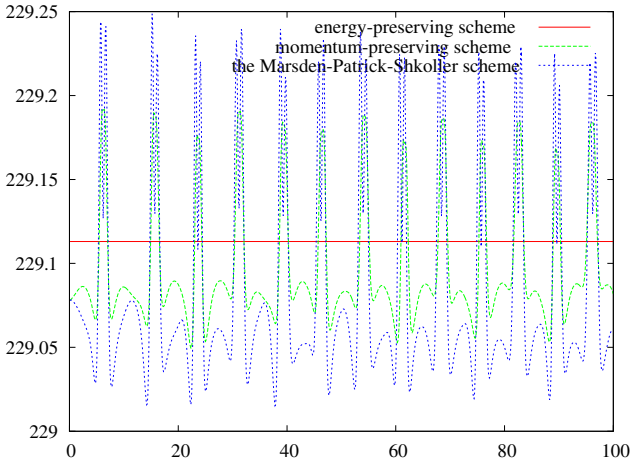

FIGURE 4. The evolutions of the total energies of the numerical solutions of the nonlinear Klein–Gordon equation (6.6).

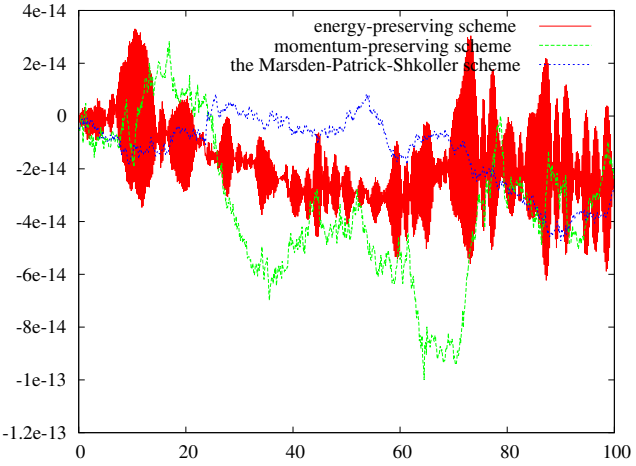

FIGURE 5. The evolutions of the total momenta of the numerical solutions of the nonlinear Klein–Gordon equation (6.6).

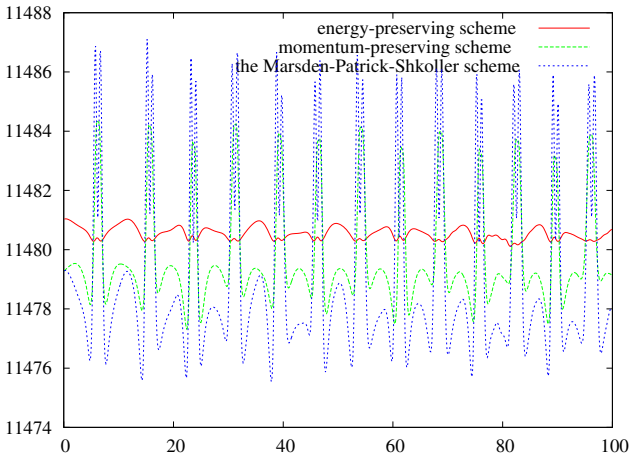

FIGURE 6. The evolutions of the total angular momenta of the numerical solutions of the nonlinear Klein–Gordon equation (6.6).

would be related to the fact that the AVF method is conjugate-symplectic of order 4 for Hamiltonian ODEs; however, we have not performed any rigorous analysis on it. Thus, the situation may depend on equations and also on choices of discrete Lagrangians.

7. Local theory of conservative schemes

In this section, we present a local theory for the energy-preserving schemes and the momentum-preserving schemes. The Noether theorem guarantees, for example, not only the global energy-conservation law but also

the local conservation law [60]

$$\begin{pmatrix} \mathrm{D}_t \\ \mathrm{D}_x \end{pmatrix} \cdot \begin{pmatrix} \mathcal{L} - u_t \dfrac{\partial \mathcal{L}}{\partial u_t} \\ -u_t \dfrac{\partial \mathcal{L}}{\partial u_x} \end{pmatrix} = 0.$$

In this section, we show that the conservative schemes presented above admit a similar discrete local conservation law.

Roughly speaking, we consider the action integral in order to apply the variational calculus, particularly the integration-by-parts formula. However, because the integration-by-parts formula is obtained by integrating the product rule $(uv)_x = u_x v + u v_x$, the local theory should be obtained by replacing the integration-by-parts formula with the product rule. The discrete product rules corresponding to the summation-by-parts formulas (3.1) and (3.2) are

$$U_j^{(n)} \left(\delta_x^+ V_j^{(n)}\right) + V_j^{(n)} \left(\delta_x^- U_j^{(n)}\right) = \delta_x^- \left(U_j^{(n)} V_{j+1}^{(n)}\right) = \delta_x^+ \left(U_{j-1}^{(n)} V_j^{(n)}\right), \tag{7.1}$$

$$U_j^{(n)} \left(\delta_t^+ V_j^{(n)}\right) + V_j^{(n)} \left(\delta_t^- U_j^{(n)}\right) = \delta_t^- \left(U_j^{(n)} V_j^{(n+1)}\right) = \delta_t^+ \left(U_j^{(n-1)} V_j^{(n)}\right). \tag{7.2}$$

Similar formulas for general difference operators are shown in Logan [46] and Miller [59].

First, we consider the energy-preserving schemes. Suppose that the given discrete Lagrangian density has the *local* symmetry at (j,n) with respect to time translation

$$\mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) = \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}),$$

instead of the *global* symmetry

$$\mathcal{L}_\mathrm{d}(j, n+z, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) = \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) \quad \text{for all } z \in \mathbb{Z}.$$

Then, we have

$$\begin{aligned} 0 &= \frac{1}{\Delta t}\left[\mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) - \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)})\right] \\ &= \frac{1}{\Delta t}\left[\mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n+1)}) - \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) - \mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n+1)}) + \mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)})\right]. \end{aligned}$$

Application of the discrete gradient (3.3) gives

$$\begin{aligned} &= \frac{1}{\Delta t}\left[\mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n+1)}) - \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)})\right] - \frac{1}{\Delta t} \bar{\nabla} \mathcal{L}_\mathrm{d} \cdot \left(\mathrm{pr}_\mathrm{d}^{(1)} (U_j^{(n+1)} - U_j^{(n)})\right)^\top \\ &= \frac{1}{\Delta t}\left[\mathcal{L}_\mathrm{d}(j, n+1, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n+1)}) - \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)})\right] \\ &\quad - \left[\delta_t^+ U_j^{(n)} \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_j^{(n+1)})}\right) + \delta_t^+ \delta_x^+ U_j^{(n)} \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_j^{(n+1)})_{x,+}}\right)\right. \\ &\quad \left. + \delta_t^+ \delta_x^- U_j^{(n)} \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_j^{(n+1)})_{x,-}}\right) + \delta_t^+ \delta_t^+ U_j^{(n)} \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_j^{(n+1)})_{t,+}}\right) + \delta_t^+ \delta_t^- U_j^{(n)} \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_j^{(n+1)})_{t,-}}\right)\right]. \end{aligned}$$

By applying the discrete product rules (7.1) and (7.2), we get

$$
\begin{aligned}
&= \frac{1}{\Delta t}\left[\mathcal{L}_{\mathrm{d}}(j,n+1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n+1)}) - \mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\right] \\
&\quad - \delta_t^+ U_j^{(n)}\left[\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})}\right) - \delta_x^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,+}}\right) - \delta_x^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,-}}\right)\right. \\
&\quad \left. - \delta_t^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,+}}\right) - \delta_t^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,-}}\right)\right] \\
&\quad - \delta_x^+\left(\left(\delta_t^+ U_j^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)},U_{j-1}^{(n+1)})_{x,+}}\right) - \delta_x^+\left(\left(\delta_t^+ U_{j-1}^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,-}}\right) \\
&\quad - \delta_t^+\left(\left(\delta_t^+ U_j^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,+}}\right) - \delta_t^+\left(\left(\delta_t^- U_j^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,-}}\right).
\end{aligned}
$$

Next, we introduce discrete counter parts of the total derivatives Δ_t^+ and Δ_x^+, which are defined by

$$
\begin{aligned}
\Delta_t^+\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) &= \frac{1}{\Delta t}\left[\mathcal{L}_{\mathrm{d}}(j,n+1,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n+1)}) - \mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\right], \\
\Delta_x^+\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) &= \frac{1}{\Delta x}\left[\mathcal{L}_{\mathrm{d}}(j+1,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_{j+1}^{(n)}) - \mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)})\right]
\end{aligned}
$$

for the discrete Lagrangian density, and by $\Delta_t^+ = \delta_t^+$ and $\Delta_x^+ = \delta_x^+$ for other quantities. Using these definitions, we get

$$
\begin{aligned}
0 = &- \delta_t^+ U_j^{(n)}\left[\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})}\right) - \delta_x^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,+}}\right) - \delta_x^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,-}}\right)\right. \\
&\left. - \delta_t^-\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,+}}\right) - \delta_t^+\left(\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,-}}\right)\right] + \Delta_t^+\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) \\
&- \Delta_x^+\left(\left(\delta_t^+ U_j^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)},U_{j-1}^{(n+1)})_{x,+}}\right) - \Delta_x^+\left(\left(\delta_t^+ U_{j-1}^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,-}}\right) \\
&- \Delta_t^+\left(\left(\delta_t^+ U_j^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,+}}\right) - \Delta_t^+\left(\left(\delta_t^- U_j^{(n)}\right)\frac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,-}}\right),
\end{aligned}
$$

which shows that the $(g_{\mathrm{d}},\bar{\nabla})$-discrete Euler–Lagrange equation satisfies the following discrete local energy conservation law:

$$
\begin{pmatrix}\Delta_t^+\\ \Delta_x^+\end{pmatrix}\cdot\begin{pmatrix}
\mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) \\
-\left(\delta_t^+ U_j^{(n)}\right)\dfrac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n-1)},U_j^{(n)})_{t,+}} - \left(\delta_t^- U_j^{(n)}\right)\dfrac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{t,-}} \\
-\left(\delta_t^+ U_j^{(n)}\right)\dfrac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_{j-1}^{(n)},U_{j-1}^{(n+1)})_{x,+}} - \left(\delta_t^+ U_{j-1}^{(n)}\right)\dfrac{\partial \mathcal{L}_{\mathrm{d}}}{\partial(U_j^{(n)},U_j^{(n+1)})_{x,-}}
\end{pmatrix} = 0.
$$

Similarly, if a discrete Lagrangian density has the local symmetry at (j,n) with respect to spatial translation

$$
\mathcal{L}_{\mathrm{d}}(j+1,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}) = \mathcal{L}_{\mathrm{d}}(j,n,\mathrm{pr}_{\mathrm{d}}^{(1)}U_j^{(n)}),
$$

we have

$$
\begin{aligned}
0 = &- \delta_x^+ U_j^{(n)} \left[\left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})} \right) - \delta_x^- \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{x,+}} \right) - \delta_x^+ \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{x,-}} \right) \right. \\
&\left. - \delta_t^- \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{t,+}} \right) - \delta_t^+ \left(\frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_j^{(n+1)})_{t,-}} \right) \right] + \Delta_x^+ \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) \\
&- \Delta_x^+ \left(\left(\delta_x^+ U_j^{(n)} \right) \frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_{j-1}^{(n)}, U_j^{(n)})_{x,+}} \right) - \Delta_x^+ \left(\left(\delta_x^- U_j^{(n)} \right) \frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{x,-}} \right) \\
&- \Delta_t^+ \left(\left(\delta_x^+ U_j^{(n)} \right) \frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n-1)}, U_{j+1}^{(n-1)})_{t,+}} \right) - \Delta_t^+ \left(\left(\delta_x^+ U_j^{(n-1)} \right) \frac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{t,-}} \right),
\end{aligned}
$$

which shows that the $(h_\mathrm{d}, \bar{\nabla})$-discrete Euler–Lagrange equation satisfies the following discrete local momentum conservation law:

$$
\begin{pmatrix} \Delta_t^+ \\ \Delta_x^+ \end{pmatrix} \cdot \begin{pmatrix} - \left(\delta_x^+ U_j^{(n)} \right) \dfrac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n-1)}, U_{j+1}^{(n-1)})_{t,+}} - \left(\delta_x^- U_j^{(n)} \right) \dfrac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{t,-}} \\ \\ \mathcal{L}_\mathrm{d}(j, n, \mathrm{pr}_\mathrm{d}^{(1)} U_j^{(n)}) \\ - \left(\delta_x^+ U_j^{(n)} \right) \dfrac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_{j-1}^{(n)}, U_j^{(n)})_{x,+}} - \left(\delta_x^- U_j^{(n)} \right) \dfrac{\partial \mathcal{L}_\mathrm{d}}{\partial (U_j^{(n)}, U_{j+1}^{(n)})_{x,-}} \end{pmatrix} = 0.
$$

8. Concluding remarks

In this paper, we have proposed a Lagrangian approach to deriving energy-preserving numerical schemes. Because our approach is a combination of the discrete gradient method and the Noether theorem in Lagrangian mechanics, it can be considered as a Lagrangian counterpart of the discrete gradient method. In our method, energy-preserving schemes are obtained as a discrete analogue of the Euler–Lagrange equation that is derived by using the symmetry of time translation of the given discrete Lagrangian density. From a practical point of view, it would be noteworthy that our approach naturally gives explicit or linearly implicit schemes in most cases, while the usual application of the discrete gradient method typically results in a nonlinear system of equations. It is also shown that the same procedure can be applied with spatial symmetry to derive momentum-preserving schemes, and the derived schemes have the corresponding local conservation law.

Finally, we make some general comments.

Other Conservation Laws and Conjugate-Symplecticity. The AVF method is shown to be conjugate-symplectic of order 4, if this method is applied to Hamiltonian ODEs [14]. Although this method can be used in our Lagrangian approach, the resulting scheme may or may not be conjugate-symplectic; thus conserved quantities other than that corresponding to the chosen symmetry may or may not be conserved. Practically, in the numerical test presented in Section 6, the energy-preserving scheme for the nonlinear Klein–Gordon equation preserves the discrete momentum and the discrete angular momentum well. This result indicates that the energy-preserving method that uses the AVF method might have conjugate-symplecticity; however, this should be investigated in future studies.

Order of Accuracy. Although the schemes shown in Section 6 are of the 2nd order in space and time, higher order schemes in the spatial direction can be obtained in a straightforward manner.

The most important tools used in our method are the summation-by-parts formula and the discrete gradient method. Therefore, to obtain higher order schemes, we need

- the summation-by-parts formula for higher order difference operators and
- a discrete gradient of higher order accuracy.

Because the former is available (see [46, 59, 70]) and the latter affects only on the temporal accuracy, we can immediately obtain spatially higher order schemes by replacing the difference operators in the discrete Lagrangian density with higher order ones, which include the pseudo-spectral difference operator.

Although, it is difficult to obtain a discrete gradient of higher order accuracy, there are some results available in the literature. For example, Matsuo proposed a high-order generalization of the Gonzalez discrete gradient [27, 51], and Hairer proposed a collocation method [32]. These methods could be combined with our method.

Multi-Dimensional Problems and Use of Nonuniform Meshes. When addressing multi-dimensional problems defined on complicated domains, use of nonuniform or triangular meshes is of great importance. If we are interested only in energy-preserving schemes, we can use these meshes, because they do not destroy the symmetry of time translation, while they destroy the spatial symmetry. The most critical step is the application of the summation-by-parts formula, or more generally the discrete Stokes theorem, on nonuniform/triangular meshes. However, because this is the same situation as in the standard (Hamiltonian-type) approach of the discrete gradient method, these formulas have been developed and are available in, for example, [58, 70].

The CFL Condition. Because the energy-preserving scheme for the nonlinear Klein–Gordon equation is explicit, step sizes must be determined so that the CFL condition is satisfied. This is inconvenient because users may be required to use a uniform temporal mesh to obtain the energy conservation law. However, as shown in Section 7, the energy-preserving scheme also satisfies the discrete local energy conservation law. This implies that different time steps can be used on each node.

Application to ODEs. Although we have focused on partial differential equations in this paper, our approach can be applied also to ordinary differential equations.

Future Studies. Possibilities for future studies include the following:

- Some other results are available that deal with symmetry of discrete systems, such as, the discrete analogues of Noether's theorem reported in [18, 19, 35, 47]. The relation of our approach to these results should be investigated.
- Backward error analysis should be applied to investigate the existence of the variational principle and other properties.
- In our approach, the schemes, and thereby their stability, depend on the discrete Lagrangian density. Hence, because in most cases, our approach gives explicit or linearly implicit multi-step schemes, we should apply the stability analysis of linear multi-step methods.
- Finally, a finite-element-type framework should be developed.

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