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An extension of the discrete variational method to nonuniform grids

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ABSTRACT

The discrete variational method is a method used to derive finite difference schemes that inherit the conservation/dissipation property of the original equations. Although this method has mainly been developed for uniform grids, we extend this method to multidimensional nonuniform meshes.

1. Introduction

For PDEs that enjoy the conservation/dissipation property, numerical schemes that inherit that property are often advantageous, in that the schemes are fairly stable and yield qualitatively better numerical solutions in practice. For example, the Cahn–Hilliard equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right), \quad (t,x) \in (0,\infty) \times (0,L), \tag{1}$$

has a dissipation property

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L \left(\frac{p}{2}u^2 + \frac{r}{4}u^4 - \frac{q}{2}\left(\frac{\partial u}{\partial x}\right)^2\right)\mathrm{d}x \leqslant 0, \quad t > 0 \tag{2}$$

under certain boundary conditions. Here $p,\ q$ and r are real parameters that satisfy $p < 0,\ q < 0$ and $r > 0$. Although the existence of the term related to the negative dispersion effect in this equation often makes naive numerical schemes unstable, some numerical schemes that are designed so that they inherit the dissipation property (2) are proved to be stable and convergent [5,8].

Recently, Furihata and Matsuo [7–9,14–17] have developed the so-called "discrete variational method" that *automatically* constructs conservative/dissipative finite difference schemes for a class of PDEs with the conservation/dissipation property

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that stems from a certain variational structure. Originally, Furihata considered two types of equations in his first paper [7]. The first is the class of equations with the form

$$\frac{\partial u}{\partial t} = (-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s}\frac{\delta G}{\delta u}, \quad s = 0,1,2,3,\ldots, \quad x \in [0,L], \tag{3}$$

where $\delta G/\delta u$ is the variational derivative, which is defined by

$$\frac{\delta G}{\delta u} = \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}. \tag{4}$$

This class of equations includes the heat equation and the Cahn–Hilliard equation. The second is the class of equations with the form

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{2s+1}\frac{\delta G}{\delta u}, \quad s = 0,1,2,3,\ldots, \quad x \in [0,L], \tag{5}$$

which includes the advection equation and the KdV equation. $G(u,u_x)$ denotes a certain energy functional, such as the Hamiltonian or free energy. The total energy of these equations is defined by

$$H(t) := \int_0^L G(u,u_x)\mathrm{d}x. \tag{6}$$

As is widely known, under certain boundary conditions, (3) has the dissipation property

$$\frac{\mathrm{d}H}{\mathrm{d}t} \leqslant 0 \tag{7}$$

and (5) has the conservation property

$$\frac{\mathrm{d}H}{\mathrm{d}t} = 0. \tag{8}$$

Furihata proposed a method to derive finite difference schemes for (3) and (5) that inherit these properties after discretization, and his method has been extended to many other equations [9,14,16,17].

Until recently, the discrete variational method has been developed on uniform meshes only. However, especially in multidimensional problems, the use of nonuniform meshes is of importance, because the restriction to uniform meshes forces the domains to be rectangles. Furthermore, even in one-dimensional cases, nonuniform meshes are often useful when solutions exhibit locally complicated behavior.

In this paper, we extend the discrete variational method to nonuniform meshes. The extension is based on the ‘‘mapping method”, where the change of coordinates plays an important role. For this reason, in the process of extension, we also show that after the change of coordinates, it remains that the conservation/dissipation property is obtained from the variational structure of the original equation.[1]

One of the most successful methods in structure preserving methods for PDEs is the mimetic approach ([1–4,11,19] and references therein). In this approach, differential operators are discretized even on unstructured meshes in a coordinate-invariant way while preserving the mass conservation, theorems of vector and tensor calculus, and the cohomology groups. Although there seem to be many similarities between the mimetic methods and our method, they are different. For example, whilst the quantities of interest in our method are from the variational structure, those in the mimetic approach are principally from geometric aspects of equations.

This paper is organized as follows.

In Section 2, we consider simple one-dimensional cases to clarify the idea of the extension, which employs the mapping method. Therefore, we briefly review the idea of the mapping method firstly in Section 2.1 and derive the conservation/dissipation property from the variational structure after the change of coordinates. In Section 2.2, we introduce a summation by parts formula on one-dimensional nonuniform grids, since it plays a very important role in the discrete variational method, similar to that of the integration by parts in conventional variational calculus. By using that formula, we define the discrete variational derivatives in Section 2.3. The dissipative and conservative schemes are defined in Sections 2.4 and 2.5, respectively.

In Section 3, we show a conservative scheme for the KdV equation as an example and give a numerical example. In Section 4, we extend the discrete variational method to multidimensional nonuniform meshes. Although we consider two-dimensional cases only for convenience of notation, the same procedure can be applied to cases greater than two dimensions. Because the integration by parts is replaced by the Gauss theorem in multidimensional cases, we show the discrete analogue of

[1] The basic idea has already been published in a Japanese paper [20].

the Gauss theorem and derive the dissipative/conservative schemes using that theorem. As an example, a dissipative scheme for the Cahn–Hilliard equation is provided in Section 5, which is accompanied by a numerical example.

The discrete variational method has been extended to equations other than those of the form (3) or (5), which include complex valued equations and nonlinear wave equations [9,14,16]. Our extension is also applicable to such equations. As an example, in Section 6, an application to a class of one-dimensional complex valued equations is described.

2. Extension to one-dimensional nonuniform grids

In this section, we extend the discrete variational method to one-dimensional nonuniform grids. We consider two classes of equations.

The first class is equations of the form (3). Equations in this class are dissipative in the following sense.

Theorem 1. (e.g. [7]). *Suppose that the boundary condition satisfies*

$$\left[\frac{\partial u}{\partial t}\frac{\partial G}{\partial u_x}\right]_0^L = 0. \tag{9}$$

Suppose also that

$$\left[\left(\frac{\partial^{p-1}}{\partial x^{p-1}}\frac{\delta G}{\delta u}\right)\left(\frac{\partial^{2s-p}}{\partial x^{2s-p}}\frac{\delta G}{\delta u}\right)\right]_0^L = 0, \quad p = 1,\ldots,s \tag{10}$$

if $s \geqslant 1$. *Then solutions of* (3) *have the dissipation property:*

$$\frac{dH}{dt} \leqslant 0, \quad H(t) = \int_0^L G(u,u_x)dx.$$

The second class is equations of the form (5). Equations in this class are conservative.

Theorem 2. (e.g. [7]). *Suppose that the boundary condition satisfies*

$$\left[\frac{\partial u}{\partial t}\frac{\partial G}{\partial u_x}\right]_0^L = 0, \quad \left[\left(\frac{\partial^s}{\partial x^s}\frac{\delta G}{\delta u}\right)^2\right]_0^L = 0.$$

Suppose also that

$$\left[\left(\frac{\partial^{p-1}}{\partial x^{p-1}}\frac{\delta G}{\delta u}\right)\left(\frac{\partial^{2s+1-p}}{\partial x^{2s+1-p}}\frac{\delta G}{\delta u}\right)\right]_0^L = 0, \quad p = 1,\ldots,s \tag{11}$$

if $s \geqslant 1$. *Then solutions of* (5) *have the conservation property:*

$$\frac{dH}{dt} = 0, \quad H(t) = \int_0^L G(u,u_x)dx = 0.$$

These theorems are proved by the following lemma:

Lemma 3. (e.g. [7]). *Suppose that a solution of* (3) or (5) *satisfies the condition*

$$\left[\frac{\partial u}{\partial t}\frac{\partial G}{\partial u_x}\right]_0^L = 0.$$

Then

$$\frac{dH}{dt} = \int_0^L \frac{\partial u}{\partial t}\frac{\delta G}{\delta u}dx. \tag{12}$$

Proof of Theorem 1. From Lemma 3 it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x = \int_0^L \frac{\partial u}{\partial t}\frac{\delta G}{\delta u}\mathrm{d}x.$$

Substituting Eq. (3) into the right-hand side and repeating applications of the integration by parts give

$$
\begin{aligned}
&= \int_0^L \left((-1)^{s+1} \left(\frac{\partial}{\partial x} \right)^{2s} \frac{\delta G}{\delta u} \right) \frac{\delta G}{\delta u} \, \mathrm{d}x \\
&= \int_0^L \left((-1)^{s+2} \left(\frac{\partial}{\partial x} \right)^{2s-1} \frac{\delta G}{\delta u} \right) \left(\frac{\partial}{\partial x} \frac{\delta G}{\delta u} \right) \mathrm{d}x + (-1)^{s+1} \left[\left(\left(\frac{\partial}{\partial x} \right)^{2s-1} \frac{\delta G}{\delta u} \right) \frac{\delta G}{\delta u} \right]_0^{x=L} \\
&\ \ \vdots \\
&= (-1)^{2s+1} \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{s} \frac{\delta G}{\delta u} \right)^2 \mathrm{d}x \leqslant 0. \qquad \square
\end{aligned}
$$

Proof of Theorem 2. From Lemma 3 it follows that

$$
\frac{\mathrm{d}}{\mathrm{d}t} \int_0^L G(u, u_x) \mathrm{d}x = \int_0^L \frac{\partial u}{\partial t} \frac{\delta G}{\delta u} \, \mathrm{d}x.
$$

Substituting Eq. (3) into the right-hand side and repeating applications of the integration by parts give

$$
\begin{aligned}
&= \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{2s+1} \frac{\delta G}{\delta u} \right) \frac{\delta G}{\delta u} \, \mathrm{d}x \\
&= -\int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{2s} \frac{\delta G}{\delta u} \right) \left(\frac{\partial}{\partial x} \frac{\delta G}{\delta u} \right) \mathrm{d}x + \left[\left(\left(\frac{\partial}{\partial x} \right)^{2s} \frac{\delta G}{\delta u} \right) \frac{\delta G}{\delta u} \right]_0^{x=L} \\
&\ \ \vdots \\
&= (-1)^s \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{s+1} \frac{\delta G}{\delta u} \right) \left(\left(\frac{\partial}{\partial x} \right)^{s} \frac{\delta G}{\delta u} \right) \mathrm{d}x \\
&= (-1)^{s+1} \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{s} \frac{\delta G}{\delta u} \right) \left(\left(\frac{\partial}{\partial x} \right)^{s+1} \frac{\delta G}{\delta u} \right) \mathrm{d}x + (-1)^s \left[\left(\frac{\partial^s}{\partial x^s} \frac{\delta G}{\delta u} \right)^2 \right]_0^L \\
&= (-1)^{s+1} \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{s} \frac{\delta G}{\delta u} \right) \left(\left(\frac{\partial}{\partial x} \right)^{s+1} \frac{\delta G}{\delta u} \right) \mathrm{d}x.
\end{aligned}
$$

It follows that

$$
\frac{\mathrm{d}}{\mathrm{d}t} \int_0^L G(u, u_x) \mathrm{d}x = (-1)^s \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{s+1} \frac{\delta G}{\delta u} \right) \left(\left(\frac{\partial}{\partial x} \right)^{s} \frac{\delta G}{\delta u} \right) \mathrm{d}x = (-1)^{s+1} \int_0^L \left(\left(\frac{\partial}{\partial x} \right)^{s} \frac{\delta G}{\delta u} \right) \left(\left(\frac{\partial}{\partial x} \right)^{s+1} \frac{\delta G}{\delta u} \right) \mathrm{d}x = 0. \qquad \square
$$

Lemma 3 is proved by a kind of calculus of variations. In fact, by the integration by parts, it is shown that

$$
\frac{\mathrm{d}}{\mathrm{d}t} \int_0^L G(u, u_x) \mathrm{d}x = \int_0^L \left(\frac{\partial u}{\partial t} \frac{\partial G}{\partial u} + \frac{\partial u_x}{\partial t} \frac{\partial G}{\partial u_x} \right) \mathrm{d}x = \int_0^L \left(\frac{\partial u}{\partial t} \frac{\partial G}{\partial u} - \frac{\partial u}{\partial t} \frac{\partial}{\partial x} \frac{\partial G}{\partial u_x} \right) \mathrm{d}x + \left[\frac{\partial u}{\partial t} \frac{\partial G}{\partial u_x} \right]_0^{x=L} = \int_0^L \frac{\partial u}{\partial t} \frac{\delta G}{\delta u} \, \mathrm{d}x.
$$

In this sense, we call Lemma 3 "the variational structure" of equations of the form (3) or (5). By discretizing this structure, the discrete variational method derives the schemes that preserve Theorems 1 or 2. It is notable that the Proof of Theorems 1 and 2 are based on the following three:

- the integration by parts;
- the variational structure, that is, the variational derivative that satisfies Lemma 3;
- the fact that the equations are written in the form (3) or (5).

The idea of the discrete variational method is to discretize these three. Thereby, in the discrete variational method,

- the summation by parts is introduced;
- the variational structure is preserved, that is, the discrete variational derivative that satisfies a discrete analogue of Lemma 3 is introduced;
- the schemes are defined using the discrete variational derivative so that they have a similar form to (3) or (5).

In the remainder of this section, we extend the discrete variational method to one-dimensional nonuniform grids, by showing that these three can be retained after discretization, even on such grids. We propose use of the mapping method, in which the spatial coordinate is transformed to so-called "computational space", which is a domain whose axis is the index of the node. With this idea in mind,

- first, in Section 2.1, we show that the conservation/dissipation properties are obtained from the variational structure even in the computational space;

and then,

- in Section 2.2, we provide a summation by parts formula on nonuniform grids;
- in Section 2.3, we introduce the discrete variational derivative on nonuniform grids and provide an analogue of Lemma 3;
- in Sections 2.4 and 2.5, we derive dissipative/conservative finite difference schemes, respectively, by using the discrete variational derivative defined in Section 2.3.

2.1. The mapping method and the dissipation/conservation properties in the computational space

We set the $N+1$ points $0 = x_0 < x_1 < x_2 < \cdots < x_N = L$ on the target domain $X = \{x | x \in [0, L]\}$. The approximated value of $u(n\Delta t, x_j)$ is denoted by $U_j^{(n)}$. Because we wish to use the mapping method, the target domain $X = \{x | x \in [0, L]\}$ is first mapped to the computational space $\Xi = \{\xi | \xi \in [0, N]\}$. We denote this map from Ξ to X by $x(\xi)$ and assume that $x(\xi)$ is a sufficiently smooth function that satisfies

$$x(j) = x_j, \quad J = \frac{\mathrm{d}x}{\mathrm{d}\xi} > 0,$$

where J is the Jacobian. In the mapping method, the differential operator $\partial/\partial x$ is discretized by approximating the right-hand side of

$$\frac{\partial}{\partial x} = \left(\frac{\mathrm{d}x}{\mathrm{d}\xi}\right)^{-1} \frac{\partial}{\partial \xi}$$

by some finite difference operators. For example, if we choose

$$\frac{\mathrm{d}x}{\mathrm{d}\xi} \simeq x_{j+1} - x_j, \quad \frac{\partial u}{\partial \xi} \simeq U_{j+1}^{(n)} - U_j^{(n)},$$

for the approximation of $\mathrm{d}x/\mathrm{d}\xi$ and $\partial u/\partial \xi$, then $\partial u/\partial x$ is discretized by

$$\frac{\partial u}{\partial x} \simeq \frac{U_{j+1}^{(n)} - U_j^{(n)}}{x_{j+1} - x_j}.$$

We are to apply this method to the discrete variational method; however, it is not obvious whether the conservation/dissipation property stems from the variational structure after the change of coordinates. Therefore, this must first be confirmed.

The transformation of (3) to the computational space results in

$$\frac{\partial u}{\partial t} = (-1)^{s+1} \left(\frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s} \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}, \quad s = 0, 1, 2, 3, \ldots,$$

where $\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}$ is the transformed variational derivative

$$\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} = \frac{\partial G}{\partial u} - J^{-1} \frac{\partial}{\partial \xi}\left(J \frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\partial G}{\partial u_x}\right).$$

This is a natural form of the variational derivative in the computational space, as later shown in Lemma 7. Since $J = \mathrm{d}x/\mathrm{d}\xi$, we can express this equation as

$$\frac{\partial u}{\partial t} = -\left(-J^{-1} \frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(-\frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1} \left(\frac{\mathrm{d}\xi}{\mathrm{d}x} J \frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1} \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}, \quad s = 0, 1, 2, 3, \ldots \tag{13}$$

Similarly (5) is transformed to

$$\frac{\partial u}{\partial t} = \left(\frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s+1} \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}, \quad s = 0, 1, 2, 3, \ldots$$

and this becomes

$$\frac{\partial u}{\partial t} = \left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}, \quad s = 0, 1, 2, 3, \ldots \tag{14}$$

Remark 1. In the above, we denote $\mathrm{d}x/\mathrm{d}\xi$ in two ways, $\mathrm{d}x/\mathrm{d}\xi$ and $J = \mathrm{d}x/\mathrm{d}\xi$. Although these are clearly the same operators, these two are distinguished, because they are discretized in different manners in the later sections. $\mathrm{d}x/\mathrm{d}\xi$ is discretized to approximate $\mathrm{d}x/\mathrm{d}\xi$ in the transformed differential operator $\mathrm{d}/\mathrm{d}x = \mathrm{d}\xi/\mathrm{d}x \cdot \mathrm{d}/\mathrm{d}\xi$, and J approximates the Jacobian in the transformed integral $\int \cdot \mathrm{d}x = \int \cdot J\,\mathrm{d}\xi$. Similarly, since $J \cdot \mathrm{d}\xi/\mathrm{d}x = 1$, it is verbose to express $J \cdot \mathrm{d}\xi/\mathrm{d}x$ and other similar terms, but we do not omit them for the same reason.

Theorems 1 and 2 in the computational space are given as follows.

Theorem 4. (Theorem 1 in the computational space). *Suppose that the boundary condition satisfies*

$$\left[\frac{\partial u}{\partial t}\frac{\partial G}{\partial u_x}\right]_{\xi=0}^{\xi=N} = 0. \tag{15}$$

Suppose also that

$$\left[\left(\left(\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\right)^{s-p}\frac{d\xi}{dx}J\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\left(\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\left(\left(\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\right)^{p-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right]_{\xi=0}^{\xi=N} = 0, \quad p = 1, \ldots, s \tag{16}$$

if $s \geqslant 1$. *Then the solutions of (13) have the dissipation property:*

$$\frac{dH_{\mathrm{cs}}}{dt} \leqslant 0, \quad H_{\mathrm{cs}}(t) = \int_0^N G(u, u_x)J\,d\xi.$$

Theorem 5. (Theorem 2 in the computational space). *Suppose that the boundary condition satisfies*

$$\left[\frac{\partial u}{\partial t}\frac{\partial G}{\partial u_x}\right]_{\xi=0}^{\xi=N} = 0, \quad \left[\left(\left(\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\right)^{s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)^2\right]_{\xi=0}^{\xi=N} = 0.$$

Suppose also that

$$\left[\left(\left(\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\right)^{p-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\left(\left(\frac{d\xi}{dx}\frac{\partial}{\partial\xi}\right)^{2s+1-p}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right]_{\xi=0}^{\xi=N} = 0, \quad p = 1, \ldots, s \tag{17}$$

if $s \geqslant 1$. *Then the solutions of (14) have the conservation property:*

$$\frac{dH_{\mathrm{cs}}}{dt} = 0, \quad H_{\mathrm{cs}}(t) = \int_0^N G(u, u_x)J\,d\xi.$$

To prove these theorems, we use the integration by parts that is transformed to the computational space.

Lemma 6. (The integration by parts in the computational space). *Let* $u(\xi)$ *and* $v(\xi)$ *be functions on* $[0, N]$ *that satisfy*

$$\left[J\frac{d\xi}{dx}uv\right]_{\xi=0}^{\xi=N} = 0. \tag{18}$$

Then

$$\int_0^N Ju\left(\frac{d\xi}{dx}\frac{dv}{d\xi}\right)d\xi = -\int_0^N Jv\left(J^{-1}\frac{d}{d\xi}\left(\frac{d\xi}{dx}Ju\right)\right)d\xi. \tag{19}$$

Proof. Lemma 6 is immediately obtained, because this is just a transformed form of the integration by parts. However, since we later discretize this lemma by the mapping method, we prove it by using calculations on the computational space only.

By applying the integration by parts with respect to ξ, we have

$$\int_0^N Ju\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}v}{\mathrm{d}\xi}\right)\mathrm{d}\xi = -\int_0^N v\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}Ju\right)\mathrm{d}\xi + \left[J\frac{\mathrm{d}\xi}{\mathrm{d}x}uv\right]_{\xi=0}^{\xi=N} = -\int_0^N v\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}Ju\right)\mathrm{d}\xi = -\int_0^N Jv\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}Ju\right)\right)\mathrm{d}\xi. \qquad \square$$

Now we show Lemma 3, the variational structure, in the computational space:

Lemma 7. *Suppose that a solution of (3) or (5) satisfies the condition*

$$\left[\frac{\partial u}{\partial t}J\frac{d\xi}{dx}\frac{\partial G}{\partial u_x}\right]_{\xi=0}^{\xi=N}=0. \tag{20}$$

Then

$$\frac{dH_{\mathrm{cs}}}{dt}=\int_0^N\frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}J\,d\xi,\quad \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}:=\frac{\partial G}{\partial u}-J^{-1}\frac{\partial}{\partial\xi}\left(J\frac{d\xi}{dx}\frac{\partial G}{\partial u_x}\right), \tag{21}$$

and $\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}$ *satisfies*

$$\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}=\frac{\delta G}{\delta u}.$$

Proof. By the chain rule, we obtain

$$\frac{\mathrm{d}H_{\mathrm{cs}}}{\mathrm{d}t}=\frac{\mathrm{d}}{\mathrm{d}t}\int_0^N GJ\,\mathrm{d}\xi=\int_0^N\left(\frac{\partial G}{\partial u}\frac{\partial u}{\partial t}+\frac{\partial G}{\partial u_x}\frac{\partial u_x}{\partial t}\right)J\,\mathrm{d}\xi=\int_0^N\frac{\partial G}{\partial u}\frac{\partial u}{\partial t}J\,\mathrm{d}\xi+\int_0^N J\left(\frac{\partial G}{\partial u_x}\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\partial u_t}{\partial\xi}\right)\mathrm{d}\xi.$$

By applying the integration by parts of the form shown in Lemma 6, we have

$$=\int_0^N\frac{\partial G}{\partial u}\frac{\partial u}{\partial t}J\,\mathrm{d}\xi-\int_0^N\frac{\partial u}{\partial t}\left(J^{-1}\frac{\partial}{\partial\xi}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\partial G}{\partial u_x}\right)\right)J\,\mathrm{d}\xi=\int_0^N\frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}J\,\mathrm{d}\xi. \tag{22}$$

For the latter part, we have

$$\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}=\frac{\partial G}{\partial u}-J^{-1}\frac{\partial}{\partial\xi}\left(J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\partial G}{\partial u_x}\right)=\frac{\partial G}{\partial u}-\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\partial}{\partial\xi}\frac{\partial G}{\partial u_x}=\frac{\partial G}{\partial u}-\frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}=\frac{\delta G}{\delta u},$$

since $J=\mathrm{d}x/\mathrm{d}\xi$. □

Thus, we have confirmed that the variational structure is retained in the computational space, so we can now proceed to prove Theorems 4 and 5.

Proof of Theorem 4. By Lemma 7, we have

$$\frac{\mathrm{d}H_{\mathrm{cs}}}{\mathrm{d}t}=\int_0^N\frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}J\,\mathrm{d}\xi.$$

Substituting Eq. (13) and application of the integration by parts in Lemma 6 give

$$=-\int_0^N\left\{\left(-J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(-\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}J\,\mathrm{d}\xi$$

$$=-\int_0^N\left\{\left(-\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}J\,\mathrm{d}\xi$$

$$=-\int_0^N\left\{\left(-J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(-\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-2}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}J\,\mathrm{d}\xi.$$

We continue in this fashion to obtain

$$=-\int_0^N\left\{\left(-J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(-\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-3}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^2\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}J\,\mathrm{d}\xi$$

$$\vdots$$

$$=-\int_0^N\left\{\left(-J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}J\,\mathrm{d}\xi$$

$$=-\int_0^N\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}J\,\mathrm{d}\xi$$

$$=-\int_0^N J\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^s\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}^2\mathrm{d}\xi\leqslant 0.$$

Proof of Theorem 5. By Lemma 7, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^N G(u,u_x)J\,\mathrm{d}\xi = \int_0^N \frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} J\,\mathrm{d}\xi.$$

Substituting Eq. (13) and application of the integration by parts in Lemma 6 give

$$= \int_0^N \left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} J\,\mathrm{d}\xi$$

$$= -\int_0^N \left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\} J\,\mathrm{d}\xi$$

$$= -\int_0^N \left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s-1}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\} J\,\mathrm{d}\xi.$$

We continue in this fashion to obtain

$$= (-1)^2\int_0^N \left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2s-2}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{2}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\} J\,\mathrm{d}\xi$$

$$\vdots$$

$$= (-1)^s\int_0^N \left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\} J\,\mathrm{d}\xi$$

$$= (-1)^{s+1}\int_0^N \left\{\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\}\left\{\left(J^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^{s}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\} J\,\mathrm{d}\xi.$$

The last equality shows that this value equals 0. □

2.2. Discrete symbols and a summation by parts formula on nonuniform grids

In this section we introduce symbols that are useful for notation and show a summation by parts formula on nonuniform grids. As in the previous section, we divide the interval $[0,L]$ into nonuniform meshes with nodes $0 = x_0 < x_1 < x_2 < \cdots < x_N = L$. The approximated value of $u(n\Delta t, x_j)$ is denoted by $U_j^{(n)}$. In what follows, δ's with suffixes denote difference operators in the computational space, that is, approximations of $\partial/\partial\xi$. For example, we write the forward difference operator in the computational space as $\delta_+ U_j^{(n)} = U_{j+1}^{(n)} - U_j^{(n)}$, the backward difference operator as $\delta_- U_j^{(n)} = U_j^{(n)} - U_{j-1}^{(n)}$ and the central difference operator as $\delta_c U_j^{(n)} = \left(U_{j+1}^{(n)} - U_{j-1}^{(n)}\right)/2$. We denote the approximated value of $\mathrm{d}x/\mathrm{d}\xi$ by $(x_\xi)_j$ or similar notations, which may be set, for example, to $(x_\xi)_j = x_{j+1} - x_j$. $(x_\xi)_j$'s are used to approximate the values that are denoted by $\mathrm{d}x/\mathrm{d}\xi$ in the previous section. We also denote the positive weights by w_j's that are defined so that $\sum_{j=0}^N w_j$ approximates the integral operator. w_j's are used to approximate the values that are denoted by J in the previous section. δ, $(x_\xi)_j$ and w_j are chosen arbitrarily, unless otherwise specified.

To discretize Lemma 6, we introduce the useful notations:

Definition 1. For a finite difference operator δ with the α-point stencil

$$\delta U_j = \sum_{k=-\alpha}^{\alpha} a_k U_{j+k},$$

we define δ^* by

$$\delta^* U_j = -\sum_{k=-\alpha}^{\alpha} a_{-k} U_{j+k}.$$

Definition 2. Let δ be a finite difference operator with the α-point stencil that is represented as

$$\delta U_j = \sum_{k=-\alpha}^{\alpha} a_k U_{j+k}.$$

Let $(x_\xi)_j$ be an arbitrarily chosen approximation of $\mathrm{d}x/\mathrm{d}\xi$ and $w_j > 0$ be the weights that are defined so that $\sum_{j=0}^N w_j$ approximates the integral operator. For any sequences U_j and V_j, we define boundary term operators $\mu_{(\pm,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\})$ by

$$\mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) := \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}_{j,k}\left(w_j(x_\xi)_j^{-1}U_jV_k\right) + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}^*_{j,k}\left(w_k(x_\xi)_k^{-1}U_kV_j\right),$$

$$\mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) := \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}_{j,k}\left(w_j(x_\xi)_j^{-1}U_jV_k\right) + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}^*_{j,k}\left(w_k(x_\xi)_k^{-1}U_kV_j\right),$$

where $\tilde{a}_{j,k}$ is defined by

$$\tilde{a}_{j,k} = \begin{cases} a_{-j+k} & (k = j-\alpha, j-\alpha+1, \ldots, j+\alpha-1, j+\alpha), \\ 0 & (\text{otherwise}) \end{cases}$$

and $\tilde{a}^*_{j,k}$ is defined corresponding to δ^* in a similar way:

$$\tilde{a}^*_{j,k} = \begin{cases} a^*_{-j+k} & (k = j-\alpha, j-\alpha+1, \ldots, j+\alpha-1, j+\alpha), \\ 0 & (\text{otherwise}), \end{cases}$$

$$a^*_k = -a_{-k}.$$

$\mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\})$ and $\mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\})$ approximate U_NV_N and $-U_0V_0$, respectively. An example is provided in Remark 2 below. We now give the summation by parts formula:

Lemma 8. *Let δ be a finite difference operator that is represented as*

$$\delta U_j = \sum_{k=-\alpha}^{\alpha} a_k U_{j+k}$$

and $(x_\xi)_j$'s be approximated values of $dx/d\xi$. For any sequences U_j and V_j that satisfy

$$\mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) + \mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) = 0, \tag{23}$$

a summation by parts formula

$$\sum_{j=0}^{N} w_jU_j((x_\xi)_j^{-1}\delta V_j) = -\sum_{j=0}^{N} w_jV_jw_j^{-1}\delta^*\left((x_\xi)_j^{-1}w_jU_j\right) \tag{24}$$

holds.

Remark 2. The condition (23) corresponds to the condition (18) in Lemma 6. To clarify this, let us consider the simplest case, where uniform grids

$$(x_\xi)_j = w_j = \Delta x$$

and the central difference operator $\delta = \delta_c$ are employed. In this case,

$$\delta U_j = \frac{1}{2}(U_{j+1} - U_{j-1}) = \sum_{k=-\alpha}^{\alpha} a_k U_{j+k}, \quad \alpha = 1, \quad a_k = \begin{cases} -1/2 & (k=-1) \\ 0 & (k=0) \\ 1/2 & (k=1) \end{cases}$$

and hence $\tilde{a}_{j,k}$ is

$$\tilde{a}_{j,k} = \begin{pmatrix} \cdots & 0, & -1/2, & 0, & 1/2, & 0, & \cdots \\ \cdots & k=j-2 & k=j-1 & k=j & k=j+1 & k=j+2 & \cdots \end{pmatrix}.$$

The central difference operator is self-adjoint in the sense that $\delta^* = \delta$ and $\tilde{a}^*_{j,k} = \tilde{a}_{j,k}$. The boundary term operators become

$$\begin{aligned}\mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) &= \sum_{j=N}^{N}\sum_{k=N+1}^{N+1}\tilde{a}_{j,k}\left(w_j(x_\xi)_j^{-1}U_jV_k\right) + \sum_{j=N}^{N}\sum_{k=N+1}^{N+1}\tilde{a}^*_{j,k}\left(w_k(x_\xi)_k^{-1}U_kV_j\right) \\ &= \tilde{a}_{N,N+1}w_N(x_\xi)_N^{-1}U_NV_{N+1} + \tilde{a}^*_{N,N+1}w_{N+1}(x_\xi)_{N+1}^{-1}U_{N+1}V_N = \frac{1}{2}(U_NV_{N+1} + U_{N+1}V_N)\end{aligned}$$

and

$$\begin{aligned}\mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) &= \sum_{j=0}^{0}\sum_{k=-1}^{-1}\tilde{a}_{j,k}\left(w_j(x_\xi)_j^{-1}U_jV_k\right) + \sum_{j=0}^{0}\sum_{k=-1}^{-1}\tilde{a}^*_{j,k}\left(w_k(x_\xi)_k^{-1}U_kV_j\right) \\ &= \tilde{a}_{0,-1}w_0(x_\xi)_0^{-1}U_0V_{-1} + \tilde{a}^*_{0,-1}w_{-1}(x_\xi)_{-1}^{-1}U_{-1}V_0 = -\frac{1}{2}(U_0V_{-1} + U_{-1}V_0).\end{aligned}$$

Thus, the left-hand side of (23) is

$$\frac{1}{2}(U_N V_{N+1} + U_{N+1} V_N) - \frac{1}{2}(U_0 V_{-1} + U_{-1} V_0),$$

which is an approximation of (18).

Remark 3. Examples for the boundary conditions that enjoy condition (23) include the Dirichlet boundary condition

$$U_j = V_j = 0 \quad \text{for all } j \text{ such that } j > N \text{ or } j < 0 \tag{25}$$

and the periodic boundary condition

$$U_{j+N+1} = U_j, \quad V_{j+N+1} = V_j, \quad (x_\xi)^{-1}_{j+N+1} = (x_\xi)^{-1}_j, \quad w_{j+N+1} = w_j \quad \text{for all } j. \tag{26}$$

These are confirmed in the following way. Under the Dirichlet boundary condition we have

$$\begin{aligned}\mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) &= \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} \tilde{a}^*_{j,k}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) \\ &= \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_j\cdot 0\Big) + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} \tilde{a}^*_{j,k}\Big(w_k(x_\xi)_k^{-1}\cdot 0\cdot V_j\Big) = 0.\end{aligned}$$

A similar calculation yields $\mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) = 0$, and combining these gives (23). In the case of the periodic boundary condition, we have

$$\begin{aligned} mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) + \mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) &= \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} \tilde{a}^*_{j,k}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) \\ &\quad + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1} \tilde{a}^*_{j,k}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) \\ &= \sum_{j=N-\alpha+1}^{N}\sum_{k=0}^{\alpha-1} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) + \sum_{j=N-\alpha+1}^{N}\sum_{k=0}^{\alpha-1} \tilde{a}^*_{j,k}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) \\ &\quad + \sum_{j=0}^{\alpha-1}\sum_{k=N-\alpha+1}^{N} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) + \sum_{j=0}^{\alpha-1}\sum_{k=N-\alpha+1}^{N} \tilde{a}^*_{j,k}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) \\ &= \sum_{j=N-\alpha+1}^{N}\sum_{k=0}^{\alpha-1} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) - \sum_{j=N-\alpha+1}^{N}\sum_{k=0}^{\alpha-1} \tilde{a}_{k,j}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) \\ &\quad + \sum_{j=0}^{\alpha-1}\sum_{k=N-\alpha+1}^{N} \tilde{a}_{j,k}\Big(w_j(x_\xi)_j^{-1}U_jV_k\Big) - \sum_{j=0}^{\alpha-1}\sum_{k=N-\alpha+1}^{N} \tilde{a}_{k,j}\Big(w_k(x_\xi)_k^{-1}U_kV_j\Big) = 0.\end{aligned}$$

Remark 4. It is common to use the inner product in order to derive summation-by-parts-type formulas [1,12,13,19]. The summation by parts formula (24) in Lemma 8 is comprehensible, if it is represented by using the inner product as well. We see it by an example where the difference operator δ is the forward difference operator $\delta = \delta_+$ and the boundary condition is given by the Dirichlet condition (25) or the periodic boundary condition (26).

Firstly, we compute the difference matrix D that represents δ. When the Dirichlet condition is imposed, we have for $j \neq N$

$$\delta U_j = U_{j+1} - U_j$$

and for $j = N$

$$\delta U_N = U_{N+1} - U_N = -U_N.$$

Therefore,

$$\begin{pmatrix} \delta U_0 \\ \delta U_1 \\ \delta U_2 \\ \vdots \\ \delta U_{N-2} \\ \delta U_{N-1} \\ \delta U_N \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & -1 & 1 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & -1 & 1 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} U_0 \\ U_1 \\ U_2 \\ \vdots \\ U_{N-2} \\ U_{N-1} \\ U_N \end{pmatrix},$$

and hence

$$D = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & -1 & 1 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & -1 & 1 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & -1 \end{pmatrix}.$$

Similarly, we have for $j \neq 0$

$$\delta^* U_j = U_j - U_{j-1}$$

and for $j = 0$

$$\delta^* U_0 = U_0 - U_{-1} = U_0,$$

and hence the difference matrix for δ^*, which is denoted as D^*, is

$$D^* = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 1 & 0 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 1 & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix}.$$

In a similar way, when the periodic boundary condition is imposed, the difference matrices become

$$D = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & -1 & 1 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & -1 & 1 \\ 1 & \cdots & \cdots & \cdots & 0 & 0 & -1 \end{pmatrix}, \quad D^* = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots & -1 \\ -1 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 1 & 0 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 1 & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix}.$$

Note that these matrices satisfy $D^* = -D^\top$.

Let matrices W and X be $W = \mathrm{diag}(w_j)$ and $X = \mathrm{diag}((x_\xi)_j)$. Let vectors $\vec{U}$ and $\vec{V}$ be $\vec{U} = (U_0, \ldots, U_N)$ and $\vec{V} = (V_0, \ldots, V_N)$. Using these notations we can rewrite

$$\sum_{j=0}^{N} w_j U_j \left((x_\xi)_j^{-1} \delta V_j \right) = \langle \vec{U}, X^{-1} D \vec{V} \rangle_W,$$

where $\langle \vec{U}, \vec{V} \rangle_W := \vec{U}^\top W \vec{V}$ is the inner product with the weight W. Since the adjoint operator of $X^{-1}D$ with respect to this inner product is $W^{-1}D^\top X^{-1}W$, we have

$$\langle \vec{U}, X^{-1} D \vec{V} \rangle_W = \langle W^{-1} D^\top X^{-1} W \vec{U}, \vec{V} \rangle_W$$

and

$$= -\langle W^{-1} (-D)^\top X^{-1} W \vec{U}, \vec{V} \rangle_W.$$

Rewriting this to the form with operators, we have

$$= -\sum_{j=0}^{N} w_j V_j w_j^{-1} \delta^* \left((x_\xi)_j^{-1} w_j U_j \right),$$

because $-D^\top$ corresponds to δ^*. This coincides with the summation by parts (24).

Furthermore, the above argument is a discrete counterpart of the fact that the transformed integration by parts (19) is expressed as

$$\left\langle u, \frac{\mathrm{d}\xi}{\mathrm{d}x} \frac{\partial v}{\partial \xi} \right\rangle_J = -\left\langle J^{-1} \frac{\partial}{\partial \xi} \left(\frac{\mathrm{d}\xi}{\mathrm{d}x} J u \right), v \right\rangle_J$$

by using the adjoint operator of the differential operator $\mathrm{d}\xi/\mathrm{d}x \cdot \partial/\partial\xi$ with respect to the inner product $\langle\cdot,\cdot\rangle_J$ whose weight is the Jacobian.

Proof of Lemma 8. In a straightforward way, we obtain

$$\begin{aligned}\sum_{j=0}^{N} w_j U_j\left((x_\xi)_j^{-1}\delta V_j\right) &= \sum_{j=0}^{N}\sum_{k=-\alpha}^{\alpha} w_j U_j (x_\xi)_j^{-1} a_k V_{j+k}\\ &= \sum_{j=0}^{N}\sum_{k=0}^{N} w_j U_j (x_\xi)_j^{-1}\tilde{a}_{j,k} V_k + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right) + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right)\\ &= \sum_{j=0}^{N}\sum_{k=0}^{N} w_k U_k (x_\xi)_k^{-1}\tilde{a}_{k,j} V_j + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right) + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right).\end{aligned}$$

Using $\tilde{a}_{j,k} = -\tilde{a}^*_{k,j}$, we obtain

$$\begin{aligned}&= -\sum_{j=0}^{N}\sum_{k=0}^{N} w_k U_k (x_\xi)_k^{-1}\tilde{a}^*_{j,k} V_j + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right) + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right)\\ &= -\sum_{j=0}^{N}\sum_{k=-\alpha}^{\alpha} w_k U_k (x_\xi)_k^{-1} a^*_k V_j + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}^*_{j,k}\left(w_k (x_\xi)_k^{-1} U_k V_j\right)\\ &\quad + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}^*_{j,k}\left(w_k (x_\xi)_k^{-1} U_k V_j\right) + \sum_{j=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right) + \sum_{j=0}^{\alpha-1}\sum_{k=-\alpha}^{-1}\tilde{a}_{j,k}\left(w_j (x_\xi)_j^{-1} U_j V_k\right)\\ &= -\sum_{j=0}^{N}\sum_{k=-\alpha}^{\alpha} w_k U_k (x_\xi)_k^{-1} a^*_k V_j + \mu_{(+,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) + \mu_{(-,\delta,(x_\xi)_j)}(\{U_j\},\{V_j\}) = -\sum_{j=0}^{N}\sum_{k=-\alpha}^{\alpha} w_k U_k (x_\xi)_k^{-1} a^*_k V_j.\end{aligned}$$

The last equality is due to (23). Rewriting this to the form with difference operators, we obtain

$$= -\sum_{j=0}^{N} w_j V_j w_j^{-1}\delta^*\left((x_\xi)_j^{-1} w_j U_j\right). \qquad \square$$

2.3. Definition of the discrete variational derivative

In this section, we introduce the discrete variational derivative on one-dimensional nonuniform grids. The discrete variational derivative will be defined by an approximation of the variational derivative in the computational space

$$\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} = \frac{\partial G}{\partial u} - J^{-1}\frac{\partial}{\partial\xi}\left(J\frac{\mathrm{d}\xi}{\mathrm{d}x}\frac{\partial G}{\partial u_x}\right).$$

Suppose that the energy functional G is given in the next form:

$$G(u,u_x) = \sum_{l=1}^{K} f_l(u) g_l(u_x), \tag{27}$$

where f_l's and g_l's are differentiable functions. We define the discrete energy functional by

$$G_{\mathrm{d}}(\vec{U}^{(n)})_j := \sum_{l=1}^{K} f_l\left(U_j^{(n)}\right)\left(\frac{1}{M_l}\sum_{m=1}^{M_l} g_l\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)}\right)\right), \tag{28}$$

where each $(x_\xi)^{-1}_{l,m,j}$ is an approximation of $(x_\xi)^{-1}$ and $\delta_{l,m}$ is a difference operator, both of which can be chosen arbitrarily. The summation with respect to m is introduced in consideration of the situation where each g_l is approximated by using more than one difference operator. An example for the KdV equation that is shown in Section 3 helps understand the meaning of this summation. We define the discrete total energy $H^{(n)}$ by

$$H^{(n)} := \sum_{j=0}^{N} w_j G_{\mathrm{d}}(\vec{U}^{(n)})_j \simeq \int_0^L G(u,u_x)\mathrm{d}x, \tag{29}$$

where w_j's are the weights that are defined so that $\sum_{j=0}^{N} w_j$ becomes an approximation of the integral.

Definition 3. We define the discrete variational derivative of $G_{\mathrm{d}}(\vec{U}^{(n)})_j$ by

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j := \sum_{l=1}^{K}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,j} - w_j^{-1}\delta^{*}_{l,m}\left((x_\xi)^{-1}_{l,m,j}w_j\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right)\right), \tag{30}$$

where

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,j} := \left(\frac{\mathrm{d}f_l}{\mathrm{d}(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{m,j}\left(\frac{g_l\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n+1)}\right)+g_l\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)}\right)}{2}\right), \tag{31}$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j} := \left(\frac{f_l\left(U_j^{(n+1)}\right)+f_l\left(U_j^{(n)}\right)}{2}\right)\left(\frac{\mathrm{d}g_l}{\mathrm{d}\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{m,j}, \tag{32}$$

$$\left(\frac{\mathrm{d}f_l}{\mathrm{d}(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{m,j} := \begin{cases}\frac{f_l\left(U_j^{(n+1)}\right)-f_l\left(U_j^{(n)}\right)}{U_j^{(n+1)}-U_j^{(n)}} & \left(U_j^{(n+1)}\neq U_j^{(n)}\right),\\ \frac{\mathrm{d}f_l}{\mathrm{d}U}\left(U_j^{(n)}\right) & (\text{otherwise}),\end{cases} \tag{33}$$

$$\left(\frac{\mathrm{d}g_l}{\mathrm{d}\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{m,j} := \begin{cases}\frac{g_l\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n+1)}\right)-g_l\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)}\right)}{(x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n+1)}-(x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)}} & \left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n+1)}\neq(x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)}\right),\\ \frac{\mathrm{d}g_l}{\mathrm{d}U_x}\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)}\right) & (\text{otherwise}).\end{cases} \tag{34}$$

The definition is chosen carefully, so that the variational structure is retained after the discretization in the sense that a discrete counterpart of Lemma 7 holds.

Lemma 9. *Suppose the condition*

$$\sum_{l=1}^{K}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\mu_{\left(+,\delta_{l,m},(x_\xi)^{-1}_{l,m,j}\right)}\left(\left\{\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right\},\left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right\}\right)\right.$$
$$\left.+\mu_{\left(-,\delta_{l,m},(x_\xi)^{-1}_{l,m,j}\right)}\left(\left\{\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right\},\left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right\}\right)\right)=0$$

is satisfied. Then

$$\frac{1}{\Delta t}(H^{(n+1)}-H^{(n)}) = \sum_{j=0}^{N}w_j\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j. \tag{35}$$

Proof. By (31) and (32) we obtain

$$\frac{1}{\Delta t}\left(H^{(n+1)}-H^{(n)}\right) = \frac{1}{\Delta t}\sum_{j=0}^{N}\sum_{l=1}^{K}w_j\left(f_l\left(U_j^{(n+1)}\right)\left(\frac{1}{M_l}\sum_{m=1}^{M_l}g_l\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n+1)}\right)\right)-f_l\left(U_j^{(n)}\right)\left(\frac{1}{M_l}\sum_{m=1}^{M_l}g_l((x_\xi)^{-1}_{l,m,j}\delta_{l,m}U_j^{(n)})\right)\right)$$
$$=\sum_{j=0}^{N}\sum_{l=1}^{K}\frac{w_j}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right)\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)},\vec{U}^{(n)}\right)}\right)_{l,m,j}\right.$$
$$\left.+\left((x_\xi)^{-1}_{l,m,j}\delta_{l,m}\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right)\right)\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}_x^{(n+1)},\vec{U}^{(n)})_x}\right)_{l,m,j}\right).$$

Applying Lemma 8, we obtain

$$= \sum_{j=0}^{N} \sum_{l=1}^{K} \frac{w_j}{M_l} \sum_{m=1}^{M_l} \left(\frac{U_j^{(n+1)} - U_j^{(n)}}{\Delta t} \right) \left(\left(\frac{\partial G_{\mathrm{d}}}{\partial (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_{l,m,j} - w_j^{-1} \delta_{l,m}^* \left((x_\xi)_{l,m,j}^{-1} w_j \left(\frac{\partial G_{\mathrm{d}}}{\partial (\vec{U}_x^{(n+1)}, \vec{U}^{(n)})_x} \right)_{l,m,j} \right) \right)$$

$$= \sum_{j=0}^{N} w_j \left(\frac{U_j^{(n+1)} - U_j^{(n)}}{\Delta t} \right) \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j . \qquad \square$$

2.4. Design of schemes for the dissipative equations

As is usual in the discrete variational method, we design schemes so that they correspond to (13) for the dissipative equations and to (14) for the conservative equations. Defining the schemes in this way allows us to obtain the dissipative/conservative property in almost the same way as Section 2.1.

We define the scheme for the dissipative equation (13) by

$$\frac{U_j^{(n+1)} - U_j^{(n)}}{\Delta t} = -\left(-w_j^{-1}\delta_s^*\right)\left(-(x_\xi)_{s,j}^{-1}\delta_{s-1}^*\right)\cdots\left(-(x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1} w_j (x_\xi)_{1,j}^{-1}\delta_1\right)\left((x_\xi)_{2,j}^{-1}\delta_2\right)\cdots\left((x_\xi)_{s-1,j}^{-1}\delta_{s-1}\right)\left((x_\xi)_{s,j}^{-1}\delta_s\right) \times \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j . \tag{36}$$

$(x_\xi)_{m,j}$ and δ_m $(m = 1, \ldots, s)$ are arbitrarily chosen depending on, for example, the accuracy of the scheme. For this scheme, we claim a discrete counterpart of Theorem 4.

Theorem 10. *Let w_j's be positive. Let $U_j^{(n)}$ be a numerical solution of the scheme (36) under the boundary condition that satisfies the assumption of Lemma 9 , and*

$$\mu_{(+,\delta_{s-p+1},w_j)}\Bigg(\left((x_\xi)_{s-p+1,j}^{-1}\delta_{s-p}^* \right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1} w_j (x_\xi)_{1,j}^{-1}\delta_1\right)\left((x_\xi)_{2,j}^{-1}\delta_2\right)\cdots\left((x_\xi)_{s-1,j}^{-1}\delta_{s-1}\right)\left((x_\xi)_{s,j}^{-1}\delta_s\right) \times \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j , (x_\xi)_{s-p+2,j}^{-1}\delta_{s-p+2}\cdots(x_\xi)_{s,j}^{-1}\delta_s \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \Bigg)$$
$$+ \mu_{(-,\delta_{s-p+1},w_j)}\Bigg(\left((x_\xi)_{s-p+1,j}^{-1}\delta_{s-p}^* \right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1} w_j (x_\xi)_{1,j}^{-1}\delta_1\right)\left((x_\xi)_{2,j}^{-1}\delta_2\right)\cdots\left((x_\xi)_{s-1,j}^{-1}\delta_{s-1}\right)\left((x_\xi)_{s,j}^{-1}\delta_s\right) \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j , (x_\xi)_{s-p+2,j}^{-1}\delta_{s-p+2}\cdots(x_\xi)_{s,j}^{-1}\delta_s \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \Bigg) = 0 \quad (p = 1, \ldots, s),$$

if $s \geqslant 1$. Then

$$\frac{1}{\Delta t}(H^{(n+1)} - H^{(n)}) \leqslant 0. \tag{37}$$

Proof. This theorem is proved in almost the same way as Theorem 4. By Lemma 9, we have

$$\frac{1}{\Delta t}(H^{(n+1)} - H^{(n)}) = \sum_{j=0}^{N} w_j \left(\frac{U_j^{(n+1)} - U_j^{(n)}}{\Delta t} \right) \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j .$$

Substituting scheme (36) and application of the summation by parts in Lemma 8 give

$$= -\sum_{j=0}^{N} w_j \left\{ \left(-w_j^{-1}\delta_s^*\right)\left(-(x_\xi)_{s,j}^{-1}\delta_{s-1}^*\right)\cdots\left(-(x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1} w_j (x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right) \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \right\} \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j$$

$$= -\sum_{j=0}^{N} w_j \left\{ \left(-(x_\xi)_{s,j}^{-1}\delta_{s-1}^*\right)\cdots\left(-(x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1} w_j (x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right) \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \right\} \left\{ w_j^{-1}\delta_s \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \right\}$$

$$= -\sum_{j=0}^{N} w_j \left\{ \left(-w_j^{-1}\delta_{s-1}^*\right)\cdots\left(-(x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1} w_j (x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right) \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \right\} \left\{ (x_\xi)_{s,j}^{-1}\delta_s \left(\frac{\delta G_{\mathrm{d}}}{\delta (\vec{U}^{(n+1)}, \vec{U}^{(n)})} \right)_j \right\}.$$

We continue in this fashion to obtain

$$= -\sum_{j=0}^{N} w_j \left\{ \left(-w_j^{-1}\delta_{s-2}^*\right)\cdots\left(-(x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}w_j(x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$\left\{ \left((x_\xi)_{s-1,j}^{-1}\delta_{s-1}\right)\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$\vdots$$
$$= -\sum_{j=0}^{N} w_j \left\{ \left(-w_j^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}w_j(x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}\left\{ \left((x_\xi)_{2,j}^{-1}\delta_2\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$= -\sum_{j=0}^{N} w_j \left\{ \left((x_\xi)_{1,j}^{-1}w_j(x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}\left\{ \left(w_j^{-1}\delta_1\right)\left((x_\xi)_{2,j}^{-1}\delta_2\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$= -\sum_{j=0}^{N} w_j \left\{ \left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}^2 \leqslant 0. \quad \square$$

2.5. Design of schemes for the conservative equations

We define the scheme for the conservative equation (14) by

$$\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t} = \left(w_j^{-1}\delta_s^*\right)\left((x_\xi)_{s,j}^{-1}\delta_{s-1}^*\right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}\delta_\mathrm{c}\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s-1,j}^{-1}\delta_{s-1}\right)\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j. \tag{38}$$

δ_c is the central difference operator. $(x_\xi)_{m,j}$ and δ_m $(m=1,\ldots,s)$ can be chosen arbitrarily. We claim a discrete counterpart of Theorem 5 for this scheme.

Theorem 11. *Let $U_j^{(n)}$ be a numerical solution of the scheme (38) under the boundary condition that satisfies the assumption of Lemma 9 and*

$$\mu_{(+,\delta_\mathrm{c},w_j)}\left(\left\{\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j\right\},\left\{\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j\right\}\right)$$
$$+\mu_{(-,\delta_\mathrm{c},w_j)}\left(\left\{\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j\right\},\left\{\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j\right\}\right) = 0. \tag{39}$$

We also assume that

$$\mu_{(+,\delta_{s-p+1},w_j)}\left(\left\{\left((x_\xi)_{s-p+1,k}^{-1}\delta_{s-p}^*\right)\left((x_\xi)_{s-p,k}^{-1}\delta_{s-p-1}^*\right)\cdots\left((x_\xi)_{2,k}^{-1}\delta_1^*\right)\left((x_\xi)_{1,k}^{-1}\delta_\mathrm{c}\right)\left((x_\xi)_{1,k}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,k}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_k\right\},\right.$$
$$\left.\left\{\left((x_\xi)_{s-p+2,j}^{-1}\delta_{s-p+2}\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j\right\}\right)$$
$$+\mu_{(-,\delta_{s-p+1},w_j)}\left(\left\{\left((x_\xi)_{s-p+1,k}^{-1}\delta_{s-p}^*\right)\left((x_\xi)_{s-p,k}^{-1}\delta_{s-p-1}^*\right)\cdots\left((x_\xi)_{2,k}^{-1}\delta_1^*\right)\left((x_\xi)_{1,k}^{-1}\delta_\mathrm{c}\right)\left((x_\xi)_{1,k}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,k}^{-1}\delta_s\right)\right.\right.$$
$$\left.\left.\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_k\right\},\left\{(x_\xi)_{s-p+2,j}^{-1}\delta_{s-p+2}\cdots(x_\xi)_{s,j}^{-1}\delta_s\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j\right\}\right) = 0 \quad (p=1,\ldots,s),$$

if $s \geqslant 1$. Then

$$\frac{1}{\Delta t}(H^{(n+1)}-H^{(n)}) = 0. \tag{40}$$

Proof. This theorem is proved in almost the same way as Theorem 5. By Lemma 9, we have

$$\frac{1}{\Delta t}(H^{(n+1)}-H^{(n)}) = \sum_{j=0}^{N} w_j\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right)\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j$$

Substituting scheme (38) and application of the summation by parts in Lemma 8 give

$$= \sum_{j=0}^{N} w_j \left\{ \left(w_j^{-1}\delta_s^*\right)\left((x_\xi)_{s,j}^{-1}\delta_{s-1}^*\right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}\delta_c\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\} \left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j$$
$$= -\sum_{j=0}^{N} w_j \left\{ \left((x_\xi)_{s,j}^{-1}\delta_{s-1}^*\right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}\delta_c\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\} \left\{ \left(w_j^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$= -\sum_{j=0}^{N} w_j \left\{ \left(w_j^{-1}\delta_{s-1}^*\right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}\delta_c\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\} \left\{ \left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}.$$

We continue in this fashion to obtain

$$= (-1)^2 \sum_{j=0}^{N} w_j \left\{ \left(w_j^{-1}\delta_{s-2}^*\right)\cdots\left((x_\xi)_{2,j}^{-1}\delta_1^*\right)\left((x_\xi)_{1,j}^{-1}\delta_c\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$\left\{ \left((x_\xi)_{s-1,j}^{-1}\delta_{s-1}\right)\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$\vdots$$
$$= (-1)^s \sum_{j=0}^{N} w_j \left\{ \left(w_j^{-1}\delta_c\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\} \left\{ \left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$= (-1)^{s+1} \sum_{j=0}^{N} w_j \left\{ \left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\} \left\{ \left(w_j^{-1}\delta_c^*\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}.$$

Since $\delta_c^* = \delta_c$, we have

$$= (-1)^{s+1} \sum_{j=0}^{N} w_j \left\{ \left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\} \left\{ \left(w_j^{-1}\delta_c\right)\left((x_\xi)_{1,j}^{-1}\delta_1\right)\cdots\left((x_\xi)_{s,j}^{-1}\delta_s\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \right\}$$
$$= 0. \qquad \square$$

Remark 5. Generally, schemes (36) and (38) yield a nonlinear system and hence a numerical solver is required. Although this increases the computational costs from naive schemes more than a little, the quasi-Newton methods solve the equations within a realistic time (see the numerical examples below). If more efficient methods are preferable, conservative/dissipative linearly implicit schemes can be constructed by modification of these schemes in a similar manner to [18].

Remark 6. Although properties such as existence, uniqueness, stability and convergence of the numerical solutions are not ensured here, they have been investigated for some specific PDEs in the case of uniform meshes (e.g. [9,10]). Therefore, the same results are expected to be obtained in a similar way for the case of nonuniform meshes.

3. An example in the one-dimensional case

In this section, we show an example for the KdV equation

$$u_t + uu_x + \gamma^2 u_{xxx} = 0. \tag{41}$$

It is well known that this equation can be written in the following form

$$u_t = \frac{\partial}{\partial x}\frac{\delta G}{\delta u}, \quad G(u,u_x) = -\frac{1}{6}u^3 - \frac{\gamma^2}{2}u_x^2. \tag{42}$$

3.1. An energy conservative scheme for the KdV equation

The energy functional $G(u,u_x)$ is written in the form of (27) with $K = 2$ and

$$f_1(u) = -\frac{1}{6}u^3, \quad f_2(u) = 1, \quad g_1(u_x) = 1, \quad g_2(u_x) = -\frac{\gamma^2}{2}u_x^2.$$

The discrete energy functional is introduced so that it corresponds to these. First, on the given nonuniform mesh, we introduce

$$(x_{\xi,+})_j := x(j+1) - x(j), \quad (x_{\xi,-})_j := x(j) - x(j-1), \quad w_j := \frac{x(j+1) - x(j-1)}{2}.$$

For $l = 1$, we set $M_1 = 1$ and approximate the term $f_1(u)g_1(u_x)$ by

$$f_1(u)g_1(u_x) = -\frac{1}{6}u^3 \simeq -\frac{1}{6}\frac{1}{M_1}\left(U_j^{(n)}\right)^3.$$

With $g_1(u_x) = 1$, the differential operator is not included in this term. Therefore, the definitions of $(x_\xi)_{1,1,j}$ and $\delta_{1,1}$ do not affect the definition of the scheme, and so we formally define them by $(x_\xi)_{1,1,j} = (x_{\xi,+})_j,\ \delta_{1,1} = \delta_+$.

The term that corresponds to $l = 2$ includes the differential operator. It is approximated using the average of the value from the forward difference δ_+ and that from the backward difference δ_-. For this reason, we set $M_2 = 2$ and

$$f_2(u)g_2(u_x) = -\frac{\gamma^2}{2}u_x^2 \simeq -\frac{\gamma^2}{2}\frac{1}{M_2}\left(\left(\frac{1}{(x_{\xi,+})_j}\delta_+ U_j^{(n)}\right)^2 + \left(\frac{1}{(x_{\xi,-})_j}\delta_- U_j^{(n)}\right)^2\right),$$

which gives

$$(x_\xi)_{2,1,j} = (x_{\xi,+})_j, \quad \delta_{2,1} = \delta_+, \quad (x_\xi)_{2,2,j} = (x_{\xi,-})_j, \quad \delta_{2,2} = \delta_-.$$

The discrete variational derivative is defined by (30)–(32):

$$\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_j = \sum_{l=1}^{2}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{\partial G_\mathrm{d}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{l,m,j} - w_j^{-1}\delta_{l,m}^{*}\left((x_\xi)_{l,m,j}^{-1}w_j\left(\frac{\partial G_\mathrm{d}}{\partial\left(\vec{U}_x^{(n+1)}, \vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right)\right),$$

$$\left(\frac{\partial G_\mathrm{d}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{1,1,j} = -\frac{1}{6}\frac{\left(U_j^{(n+1)}\right)^3 - \left(U_j^{(n)}\right)^3}{U_j^{(n+1)} - U_j^{(n)}} = -\frac{\left(U_j^{(n+1)}\right)^2 + U_j^{(n+1)}U_j^{(n)} + \left(U_j^{(n)}\right)^2}{6},$$

$$\left(\frac{\partial G_\mathrm{d}}{\partial\left(\vec{U}_x^{(n+1)}, \vec{U}_x^{(n)}\right)}\right)_{1,1,j} = -\frac{1}{6}\left(\frac{\left(U_j^{(n+1)}\right)^3 + \left(U_j^{(n)}\right)^3}{2}\right)\left(\frac{1-1}{(x_\xi)_{1,1,j}^{-1}\delta_{1,1}U_j^{(n+1)} - (x_\xi)_{1,1,j}^{-1}\delta_{1,1}U_j^{(n)}}\right) = 0,$$

$$\left(\frac{\partial G_\mathrm{d}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{2,1,j} = -\frac{\gamma^2}{2}\left(\frac{1-1}{U_j^{(n+1)} - U_j^{(n)}}\right)\left(\frac{\left((x_\xi)_{2,1,j}^{-1}\delta_{2,1}U_j^{(n+1)}\right)^2 + \left((x_\xi)_{2,1,j}^{-1}\delta_{2,1}U_j^{(n)}\right)^2}{2}\right) = 0,$$

$$\left(\frac{\partial G_\mathrm{d}}{\partial\left(\vec{U}_x^{(n+1)}, \vec{U}_x^{(n)}\right)}\right)_{2,1,j} = -\frac{\gamma^2}{2}\left(\frac{1+1}{2}\right)\left(\frac{\left((x_\xi)_{2,1,j}^{-1}\delta_{2,1}U_j^{(n+1)}\right)^2 - \left((x_\xi)_{2,1,j}^{-1}\delta_{2,1}U_j^{(n)}\right)^2}{(x_\xi)_{2,1,j}^{-1}\delta_{2,1}U_j^{(n+1)} - (x_\xi)_{2,1,j}^{-1}\delta_{2,1}U_j^{(n)}}\right) = -\frac{\gamma^2}{2}(x_{\xi,+})_j^{-1}\delta_+\left(U_j^{(n+1)} + U_j^{(n)}\right),$$

$$\left(\frac{\partial G_\mathrm{d}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{2,2,j} = -\frac{\gamma^2}{2}\left(\frac{1-1}{U_j^{(n+1)} - U_j^{(n)}}\right)\left(\frac{\left((x_\xi)_{2,2,j}^{-1}\delta_{2,2}U_j^{(n+1)}\right)^2 + \left((x_\xi)_{2,2,j}^{-1}\delta_{2,2}U_j^{(n)}\right)^2}{2}\right) = 0,$$

$$\left(\frac{\partial G_\mathrm{d}}{\partial\left(\vec{U}_x^{(n+1)}, \vec{U}_x^{(n)}\right)}\right)_{2,2,j} = -\frac{\gamma^2}{2}\left(\frac{1+1}{2}\right)\left(\frac{\left((x_\xi)_{2,2,j}^{-1}\delta_{2,2}U_j^{(n+1)}\right)^2 - \left((x_\xi)_{2,2,j}^{-1}\delta_{2,2}U_j^{(n)}\right)^2}{(x_\xi)_{2,2,j}^{-1}\delta_{2,2}U_j^{(n+1)} - (x_\xi)_{2,2,j}^{-1}\delta_{2,2}U_j^{(n)}}\right) = -\frac{\gamma^2}{2}(x_{\xi,-})_j^{-1}\delta_-\left(U_j^{(n+1)} + U_j^{(n)}\right).$$

The scheme is defined by (38) with $s = 0$

$$\frac{U_j^{(n+1)} - U_j^{(n)}}{\Delta t} = w_j^{-1}\delta_\mathrm{c}\left(\frac{\delta G_\mathrm{d}}{\delta(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_j.$$

By substituting the discrete variational derivative, we obtain the scheme

$$\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}=w_j^{-1}\delta_c\left\{\frac{\left(U_j^{(n+1)}\right)^2+U_j^{(n+1)}U_j^{(n)}+\left(U_j^{(n)}\right)^2}{6}\right.$$
$$\left.+\frac{\gamma^2}{4}\left(\left(w_j^{-1}\delta_-\right)\left((x_{\xi,+})_j^{-1}w_j(x_{\xi,+})_j^{-1}\delta_+\right)\left(U_j^{(n+1)}+U_j^{(n)}\right)+\left(w_j^{-1}\delta_+\right)\left((x_{\xi,-})_j^{-1}w_j(x_{\xi,-})_j^{-1}\delta_-\right)\left(U_j^{(n+1)}+U_j^{(n)}\right)\right)\right\}. \tag{43}$$

This scheme is the same as that by Furihata [7] if the nodes are placed uniformly.

3.2. Numerical example

We solved the KdV equation numerically using scheme (43). The problem is set in the same way as the famous experiment by Zabusky and Kruskal [21], where the domain is set to $[0,2]$ and the initial condition is given by

$$u(0,x)=\cos(\pi x).$$

The boundary condition is periodic. We set $\gamma = 0.022$. Zabusky and Kruskal reported that the solution exhibits a sharp slope near $x = 0.5$ at $t = 1/\pi$. We compare the numerical solutions that are obtained using a uniform mesh and a nonuniform mesh, as shown in Fig. 1, in which the nodes are concentrated near $x = 0.5$. Both meshes consist of 55 nodes. The spatial intervals of the nonuniform mesh are approximately 0.005 and 0.06 at the finest coarsest areas, respectively. The time interval is $\Delta t = 0.0001$. We used MINPACK to solve the nonlinear systems. The total computation time is almost the same for each case and is approximately 10 seconds with a 3.00 GHz Intel Core2 Duo CPU (just one core is used).

The numerical solutions at $t = 0.44$ using the uniform mesh and the nonuniform mesh are shown in Figs. 2 and 3, respectively. The solid line in each figure is a numerical result obtained using a finer uniform mesh that consists of 400 nodes. By comparing these two figures, we deduce that the use of the nonuniform mesh can improve the numerical solution in the sense that the oscillation near $x = 0.6$ can be captured on the nonuniform mesh, unlike that for the uniform mesh.

The time evolution of the energy for the case where the nonuniform mesh is employed is shown in Fig. 4, which confirms the energy conservation property stated in Theorem 11.

4. Extension to multidimensional nonuniform grids

In this section, we extend the discrete variational method to multidimensional nonuniform grids. In multidimensional cases, notation becomes extremely complicated. For this reason, we consider only the two-dimensional case, although extensions to problems greater than two dimensions are obtained in the same manner.

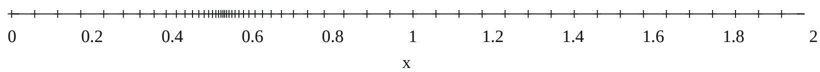


Fig. 1. The nonuniform mesh used in Section 3.2.

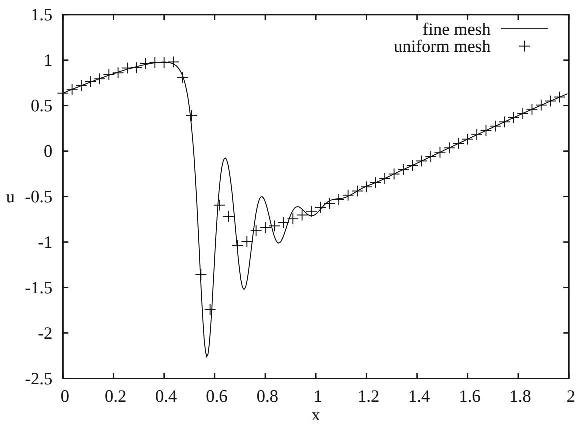


Fig. 2. Numerical solution at $t = 0.44$ using the uniform mesh. The solid line is the solution obtained using a finer uniform mesh, which consists of 400 nodes.

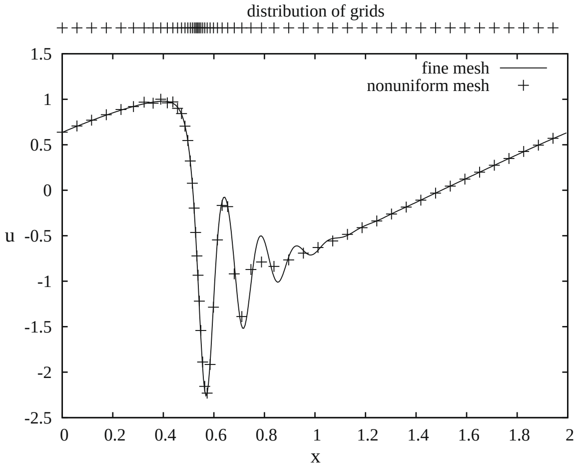


Fig. 3. Numerical solution at $t = 0.44$ using the nonuniform mesh. The solid line is the solution obtained using a finer uniform mesh, which consists of 400 nodes.

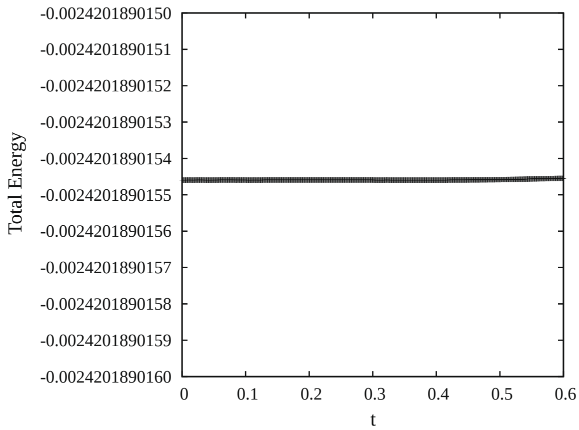


Fig. 4. Time evolution of the total energy when the nonuniform mesh is employed.

4.1. Target equations

Here we consider the following equations on a two-dimensional domain Ω, which are two-dimensional analogues of the equations considered in the previous sections. We assume that a sufficiently smooth homeomorphism exists between Ω and the computational space.

For the two-dimensional cases, the variational derivative is defined by

$$\frac{\delta G}{\delta u} := \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial G}{\partial u_y}.$$

The dissipative equations that correspond to (3) become

$$\frac{\partial u}{\partial t} = (-1)^{s+1}\left(\frac{\partial^{2s}}{\partial x^{2s}} + \frac{\partial^{2s}}{\partial y^{2s}}\right)\frac{\delta G}{\delta u}, \quad (t,x,y) \in (0,\infty)\times\Omega, \quad s = 0,1. \tag{44}$$

We consider only $s = 0, 1$, because few equations exist with $s > 1$ in multidimensional cases. Equations of this form enjoy the dissipation property.

Theorem 12. *Suppose that the boundary condition satisfies*

$$\int_{\partial\Omega} \frac{\partial u}{\partial t}\left(\frac{\partial G}{\partial u_x}, \frac{\partial G}{\partial u_y}\right)^{\top} \cdot n\, ds = 0, \tag{45}$$

where $n = (n_1, n_2)^\top$ is the unit normal vector to the boundary and ds is the area element. Suppose also that

$$\int_{\partial\Omega} \frac{\delta G}{\delta u}\left(\nabla \frac{\delta G}{\delta u} \cdot n\right) ds = 0 \tag{46}$$

if $s = 1$. Then the solutions of (44) have the dissipation property:

$$\frac{dH}{dt} \leqslant 0, \quad H(t) = \int_\Omega G(u, u_x, u_y)\,dx\,dy.$$

The conservative equations that correspond to (5) become

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)\frac{\delta G}{\delta u}, \quad (t, x, y) \in (0, \infty) \times \Omega. \tag{47}$$

Theorem 13. *Suppose that the boundary condition satisfies*

$$\int_{\partial\Omega} \frac{\partial u}{\partial t}\left(\frac{\partial G}{\partial u_x}, \frac{\partial G}{\partial u_y}\right)^\top \cdot n\,ds = 0, \quad \int_{\partial\Omega}\left(\frac{\delta G}{\delta u}\right)^2 (n_1 + n_2) ds = 0, \tag{48}$$

where $n = (n_1, n_2)^\top$ is the unit normal vector to the boundary and ds is the area element. Then the solutions of (47) have the conservation property:

$$\frac{dH}{dt} = 0, \quad H(t) = \int_\Omega G(u, u_x, u_y)\,dx\,dy. \tag{49}$$

We show "the variational structure" of these equations:

Lemma 14. *Suppose that a solution of (44) or (47) satisfies the condition*

$$\int_{\partial\Omega} \frac{\partial u}{\partial t}\left(\frac{\partial G}{\partial u_x}, \frac{\partial G}{\partial u_y}\right)^\top \cdot n\,ds = 0. \tag{50}$$

Then

$$\frac{dH}{dt} = \int_\Omega \frac{\partial u}{\partial t}\frac{\delta G}{\delta u}\,dx\,dy. \tag{51}$$

Proof. By the Gauss theorem, we have

$$\begin{aligned}\frac{dH}{dt} &= \frac{d}{dt}\int_\Omega G(u, u_x, u_y)\,dx\,dy = \int_\Omega \left(\frac{\partial G}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial u_x}\frac{\partial u_x}{\partial t} + \frac{\partial G}{\partial u_y}\frac{\partial u_y}{\partial t}\right) dx\,dy \\ &= \int_\Omega \left(\frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial G}{\partial u_y}\right)\frac{\partial u}{\partial t}\,dx\,dy + \int_{\partial\Omega}\frac{\partial u}{\partial t}\left(\frac{\partial G}{\partial u_x}, \frac{\partial G}{\partial u_y}\right)^\top \cdot n\,ds = \int_\Omega \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\,dx\,dy. \qquad \square\end{aligned}$$

Proof of Theorem 12. Applying Lemma 14 gives

$$\frac{dH}{dt} = \int_\Omega \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\,dx\,dy.$$

In the case where $s = 0$, substituting the equation yields

$$\int_\Omega \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\,dx\,dy = -\int_\Omega \left(\frac{\delta G}{\delta u}\right)^2 dx\,dy \leqslant 0.$$

In the case where $s = 1$, applying the Gauss theorem one more time gives

$$\begin{aligned}\int_\Omega \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\,dx\,dy &= \int_\Omega \left(\frac{\delta G}{\delta u}\right)\left(\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\frac{\delta G}{\delta u}\right) dx\,dy = -\int_\Omega \left(\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)\frac{\delta G}{\delta u}\right)^2 dx\,dy + \int_{\partial\Omega}\frac{\delta G}{\delta u}\left(\nabla\frac{\delta G}{\delta u}\cdot n\right) ds \\ &= -\int_\Omega \left(\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)\frac{\delta G}{\delta u}\right)^2 dx\,dy \leqslant 0. \qquad \square\end{aligned}$$

Proof of Theorem 13. Applying Lemma 14 gives

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \int_\Omega \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\,\mathrm{d}x\,\mathrm{d}y.$$

Substituting the equation and applying the Gauss theorem yield

$$\begin{aligned} &= \int_\Omega \left(\frac{\delta G}{\delta u}\right)\left(\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)\frac{\delta G}{\delta u}\right)\mathrm{d}x\,\mathrm{d}y \\ &= -\int_\Omega \left(\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)\frac{\delta G}{\delta u}\right)\left(\frac{\delta G}{\delta u}\right)\mathrm{d}x\,\mathrm{d}y + \int_{\partial\Omega}\left(\frac{\delta G}{\delta u}\right)^2 (n_1+n_2)\mathrm{d}s \\ &= -\int_\Omega \left(\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)\frac{\delta G}{\delta u}\right)\left(\frac{\delta G}{\delta u}\right)\mathrm{d}x\,\mathrm{d}y, \end{aligned}$$

and hence

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega G(u,u_x,u_y)\mathrm{d}x\,\mathrm{d}y = 0. \qquad \square$$

4.2. The dissipation/conservation properties in the computational space

In this section, we extend the discrete variational method to multidimensional nonuniform grids, such as that shown in Fig. 5. We assume that the number of nodes is $(N+1)\times(M+1)$. As in the one-dimensional case, we use the mapping method. Firstly, we describe the proofs of the conservation/dissipation properties in the computational space with the coordinates (ξ,η), and then define the discrete variational derivative and the schemes.

In the computational space, the partial derivatives are transformed to

$$\frac{\partial v}{\partial x} = J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)v, \quad \frac{\partial v}{\partial y} = J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)v, \tag{52}$$

where v is a smooth function and J is the Jacobian

$$J = \det\begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}\end{pmatrix}.$$

Note that the partial derivatives are also written as

$$\frac{\partial v}{\partial x} = J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}v\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}v\right)\right), \quad \frac{\partial v}{\partial y} = J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}v\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}v\right)\right), \tag{53}$$

since $x_{\xi\eta} = x_{\eta\xi},\ y_{\xi\eta} = y_{\eta\xi}$.

Using these formulas, we rewrite the equations in the following forms that are suitable for the discretizations. The dissipative equations (44) are transformed to

$$\frac{\partial u}{\partial t} = -\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}, \tag{54}$$

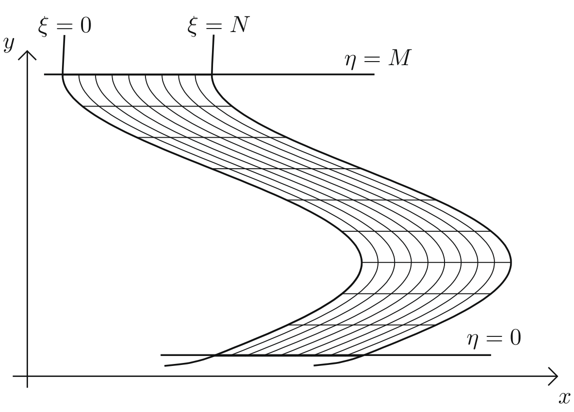


Fig. 5. An example of nonuniform grids in $\mathbb{R}^2$.

if $s = 0$, and to

$$\frac{\partial u}{\partial t} = J^{-1}\left\{\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right)\right\}$$
$$+ J^{-1}\left\{\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\left(J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\left(J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right)\right\}, \tag{55}$$

if $s = 1$. The conservative equation (47) are transformed to

$$\frac{\partial u}{\partial t} = \frac{1}{2}\left[\left\{J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} + J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right\} + \left\{J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right)\right.\right.$$
$$\left.\left. + J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\right)\right)\right\}\right]. \tag{56}$$

$(\delta G/\delta u)_{\mathrm{cs}}$ is the transformed variational derivative

$$\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} := \frac{\partial G}{\partial u} - \left(J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\frac{\partial G}{\partial u_x}\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\frac{\partial G}{\partial u_x}\right)\right) + J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\frac{\partial G}{\partial u_y}\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\frac{\partial G}{\partial u_y}\right)\right)\right). \tag{57}$$

Theorems 12 and 13 are transformed to the following.

Theorem 15. *Suppose that the boundary condition satisfies*

$$\left[\int_0^M \frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u_x}\frac{\partial y}{\partial \eta} - \frac{\delta G}{\delta u_y}\frac{\partial x}{\partial \eta}\right)d\eta\right]_{\xi=0}^{\xi=N} + \left[\int_0^N \frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u_x}\frac{\partial y}{\partial \xi} - \frac{\delta G}{\delta u_y}\frac{\partial x}{\partial \xi}\right)d\xi\right]_{\eta=M}^{\eta=0} = 0. \tag{58}$$

Suppose also that

$$\left[\int_0^M \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\frac{\partial y}{\partial \eta} - J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\frac{\partial x}{\partial \eta}\right)d\eta\right]_{\xi=0}^{\xi=N}$$
$$+ \left[\int_0^N \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\frac{\partial y}{\partial \xi} - J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}\frac{\partial x}{\partial \xi}\right)d\xi\right]_{\eta=M}^{\eta=0} = 0, \tag{59}$$

if $s = 1$. *Then the solutions of* (54) *or* (55) *have the dissipation property:*

$$\frac{dH_{\mathrm{cs}}}{dt} \leqslant 0, \quad H_{\mathrm{cs}}(t) = \int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N} G(u, u_x, u_y)J\,d\xi\,d\eta.$$

Theorem 16. *Suppose that the boundary condition satisfies*

$$\left[\int_0^M \frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u_x}\frac{\partial y}{\partial \eta} - \frac{\delta G}{\delta u_y}\frac{\partial x}{\partial \eta}\right)d\eta\right]_{\xi=0}^{\xi=N} + \left[\int_0^N \frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u_x}\frac{\partial y}{\partial \xi} - \frac{\delta G}{\delta u_y}\frac{\partial x}{\partial \xi}\right)d\xi\right]_{\eta=M}^{\eta=0}$$
$$= 0, \quad \left[\int_0^M \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}^2\left(\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\right)d\eta\right]_{\xi=0}^{\xi=N} + \left[\int_0^N \left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}^2\left(\frac{\partial y}{\partial \xi} - \frac{\partial x}{\partial \xi}\right)d\xi\right]_{\eta=M}^{\eta=0} = 0. \tag{60}$$

Then the solutions of (56) *have the conservation property:*

$$\frac{dH_{\mathrm{cs}}}{dt} = 0, \quad H_{\mathrm{cs}}(t) = \int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N} G(u, u_x, u_y)J\,d\xi\,d\eta.$$

Remark 7. Conditions (59) and (60) in the computational space correspond to the conditions (46) and (48) in the real space, respectively. The curves that are defined by $\xi = (\text{const.})$ or $\eta = (\text{const.})$ form the boundary $\partial\Omega$. Moreover, $\mathrm{d}s = \pm \mathrm{d}\eta$ and $n = \pm(\partial y/\partial \eta, -\partial x/\partial \eta)^\top$ on $\xi = (\text{const.})$, and $\mathrm{d}s = \pm \mathrm{d}\xi$ and $n = \pm(\partial y/\partial \xi, -\partial x/\partial \xi)^\top$ on $\eta = (\text{const.})$, which show the equivalence between them.

For the proofs of these theorems, we prepare the Gauss theorem transformed to the computational space.

Lemma 17. *Let* $u,\ v_1,\ v_2$ *be smooth functions that satisfy*

$$\left[\int_0^M u\left(v_1\frac{\partial y}{\partial \eta} - v_2\frac{\partial x}{\partial \eta}\right)d\eta\right]_{\xi=0}^{\xi=N} + \left[\int_0^N u\left(v_1\frac{\partial y}{\partial \xi} - v_2\frac{\partial x}{\partial \xi}\right)d\xi\right]_{\eta=M}^{\eta=0} = 0. \tag{61}$$

Then

$$\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\left(v_1 J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi}-\frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)u+v_2 J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta}-\frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)u\right)J\,d\xi\,d\eta$$
$$=-\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\left(J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}v_1\right)-\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}v_1\right)\right)+J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}v_2\right)-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}v_2\right)\right)\right)J\,d\xi\,d\eta.$$

Proof. We can obtain this lemma by application of the integration by parts in the ξ and the η directions. In fact,

$$\begin{aligned}
&\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\left(v_1 J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi}-\frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)u+v_2 J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta}-\frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)u\right)J\,\mathrm{d}\xi\,\mathrm{d}\eta\\
&=\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\left(v_1\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi}-\frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)u+v_2\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta}-\frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)u\right)\mathrm{d}\xi\,\mathrm{d}\eta\\
&=-\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}v_1\right)\mathrm{d}\xi\,\mathrm{d}\eta+\left[\int_0^M\frac{\partial y}{\partial \eta}uv_1\,\mathrm{d}\eta\right]_{\xi=0}^{\xi=N}\\
&\quad+\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}v_1\right)\mathrm{d}\xi\,\mathrm{d}\eta-\left[\int_0^N\frac{\partial y}{\partial \xi}uv_1\,\mathrm{d}\xi\right]_{\eta=0}^{\eta=M}\\
&\quad-\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}v_2\right)\mathrm{d}\xi\,\mathrm{d}\eta+\left[\int_0^N\frac{\partial x}{\partial \xi}uv_2\,\mathrm{d}\xi\right]_{\eta=0}^{\eta=M}\\
&\quad+\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}v_2\right)\mathrm{d}\xi\,\mathrm{d}\eta-\left[\int_0^M\frac{\partial x}{\partial \eta}uv_2\,\mathrm{d}\eta\right]_{\xi=0}^{\xi=N}\\
&=-\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\left(J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}v_1\right)-\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}v_1\right)\right)+J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}v_2\right)-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}v_2\right)\right)\right)J\,\mathrm{d}\xi\,\mathrm{d}\eta\\
&\quad+\left[\int_0^M u\left(v_1\frac{\partial y}{\partial \eta}-v_2\frac{\partial x}{\partial \eta}\right)\mathrm{d}\eta\right]_{\xi=0}^{\xi=N}+\left[\int_0^N u\left(v_1\frac{\partial y}{\partial \xi}-v_2\frac{\partial x}{\partial \xi}\right)\mathrm{d}\xi\right]_{\eta=M}^{\eta=0}\\
&=-\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}u\left(J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}v_1\right)-\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}v_1\right)\right)+J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}v_2\right)-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}v_2\right)\right)\right)J\,\mathrm{d}\xi\,\mathrm{d}\eta.\qquad\square
\end{aligned}$$

Next, we transform Lemma 14.

Lemma 18. *Suppose that a solution of (44) or (47) satisfies the condition*

$$\left[\int_0^M u_t\left(\frac{\delta G}{\delta u_x}\frac{\partial y}{\partial \eta}-\frac{\delta G}{\delta u_y}\frac{\partial x}{\partial \eta}\right)d\eta\right]_{\xi=0}^{\xi=N}+\left[\int_0^N u_t\left(\frac{\delta G}{\delta u_x}\frac{\partial y}{\partial \xi}-\frac{\delta G}{\delta u_y}\frac{\partial x}{\partial \xi}\right)d\xi\right]_{\eta=M}^{\eta=0}=0.$$

Then

$$\frac{dH}{dt}=\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}J\,d\xi\,d\eta. \tag{62}$$

Proof. By the chain rule, we have

$$\begin{aligned}
\frac{\mathrm{d}H}{\mathrm{d}t}&=\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega G\,\mathrm{d}x\,\mathrm{d}y=\int_\Omega\left(\frac{\partial G}{\partial u}\frac{\partial u}{\partial t}+\frac{\partial G}{\partial u_x}\frac{\partial u_x}{\partial t}+\frac{\partial G}{\partial u_y}\frac{\partial u_y}{\partial t}\right)\mathrm{d}x\,\mathrm{d}y\\
&=\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\frac{\partial G}{\partial u}\frac{\partial u}{\partial t}J\,\mathrm{d}\xi\,\mathrm{d}\eta+\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\left(\frac{\partial G}{\partial u_x}J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial u_t}{\partial \xi}-\frac{\partial y}{\partial \xi}\frac{\partial u_t}{\partial \eta}\right)+\frac{\partial G}{\partial u_y}J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial u_t}{\partial \eta}-\frac{\partial x}{\partial \eta}\frac{\partial u_t}{\partial \xi}\right)\right)J\,\mathrm{d}\xi\,\mathrm{d}\eta.
\end{aligned} \tag{63}$$

By applying the transformed Gauss theorem shown in Lemma 17, we obtain

$$\begin{aligned}
&=\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\frac{\partial G}{\partial u}\frac{\partial u}{\partial t}J\,\mathrm{d}\xi\,\mathrm{d}\eta-\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\frac{\partial u}{\partial t}\left\{J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\frac{\partial G}{\partial u_x}\right)-\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\frac{\partial G}{\partial u_x}\right)\right)+J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\frac{\partial G}{\partial u_y}\right)-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\frac{\partial G}{\partial u_y}\right)\right)\right\}J\,\mathrm{d}\xi\,\mathrm{d}\eta\\
&=\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\frac{\partial u}{\partial t}\left\{\frac{\partial G}{\partial u}-\left(J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\frac{\partial G}{\partial u_x}\right)-\frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\frac{\partial G}{\partial u_x}\right)\right)+J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\frac{\partial G}{\partial u_y}\right)-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\frac{\partial G}{\partial u_y}\right)\right)\right)\right\}J\,\mathrm{d}\xi\,\mathrm{d}\eta\\
&=\int_{\eta=0}^{\eta=M}\int_{\xi=0}^{\xi=N}\frac{\partial u}{\partial t}\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}}J\,\mathrm{d}\xi\,\mathrm{d}\eta.\qquad\square
\end{aligned}$$

Now we can prove Theorems 15 and 16.

Proof of Theorem 15. By Lemma 18, we have

$$\frac{dH}{dt} = \int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \frac{\partial u}{\partial t} \left(\frac{\delta G}{\delta u}\right)_{cs} J\, d\xi\, d\eta. \tag{64}$$

In the case of $s = 0$, substituting Eq. (54) yields

$$(64) = -\int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \left(\frac{\delta G}{\delta u}\right)_{cs}^{2} J\, d\xi\, d\eta \leqslant 0.$$

In the case of $s = 1$, substituting Eq. (55) and applying the Gauss theorem in the form of Lemma 17 yield

$$\begin{aligned}(64) = &\int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \left[J^{-1}\left\{ \frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right)\right\}\right. \\ &\left. + J^{-1}\left\{ \frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\left(J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\left(J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right)\right\}\right]\left(\frac{\delta G}{\delta u}\right)_{cs} J\, d\xi\, d\eta \\ = &-\int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \left\{ \left(J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right)^{2} + \left(J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right)^{2}\right\} J\, d\xi\, d\eta \leqslant 0. \qquad \square\end{aligned}$$

Proof of Theorem 16. Applying Lemma 18 we have

$$\frac{dH}{dt} = \int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \frac{\partial u}{\partial t} \left(\frac{\delta G}{\delta u}\right)_{cs} J\, d\xi\, d\eta.$$

Substituting Eq. (56) yields

$$\begin{aligned}= &\int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \frac{1}{2}\left[\left\{ J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{cs} + J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right\}\right. \\ &\left. \times \left\{ J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\left(\frac{\delta G}{\delta u}\right)_{cs}\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right) + J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\left(\frac{\delta G}{\delta u}\right)_{cs}\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right)\right\}\right]\left(\frac{\delta G}{\delta u}\right)_{cs} J\, d\xi\, d\eta.\end{aligned}$$

Application of Lemma 17 yields

$$\begin{aligned}= -&\int_{\eta=0}^{\eta=M} \int_{\xi=0}^{\xi=N} \frac{1}{2}\left[\left\{ J^{-1}\left(\frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial \eta}\left(\frac{\delta G}{\delta u}\right)_{cs}\right) - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial \xi}\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right) + J^{-1}\left(\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial \xi}\left(\frac{\delta G}{\delta u}\right)_{cs}\right) - \frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial \eta}\left(\frac{\delta G}{\delta u}\right)_{cs}\right)\right)\right\}\right. \\ &\left. + \left\{ J^{-1}\left(\frac{\partial y}{\partial \eta}\frac{\partial}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial}{\partial \eta}\right)\left(\frac{\delta G}{\delta u}\right)_{cs} + J^{-1}\left(\frac{\partial x}{\partial \xi}\frac{\partial}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial}{\partial \xi}\right)\left(\frac{\delta G}{\delta u}\right)_{cs}\right\}\right]\left(\frac{\delta G}{\delta u}\right)_{cs} J\, d\xi\, d\eta,\end{aligned}$$

and hence, this equals 0. □

4.3. The discrete Gauss theorem on multidimensional nonuniform grids

In this section, we provide a discrete counterpart of the Gauss theorem. As is seen in the Proof of Lemma 17, the Gauss theorem in the computational space is obtained simply by applying the integration by parts in the ξ and η directions. Therefore, the discrete Gauss theorem is obtained by applying the summation by parts in each direction.

First, similarly to the one-dimensional case, we introduce a boundary term operator to simplify notation.

Definition 4. Let δ_ξ and δ_η be finite difference operators in the ξ and η directions, respectively:

$$\delta_\xi U_{i,j} = \sum_{k=-\alpha}^{\alpha} a_k U_{i+k,j}, \quad \delta_\eta U_{i,j} = \sum_{k=-\beta}^{\beta} b_k U_{i,j+k}.$$

We define $\tilde{a}_{i,k},\ \tilde{a}^*_{i,k},\ \tilde{b}_{j,k}$ and $\tilde{b}^*_{j,k}$ by

$$\begin{aligned}\tilde{a}_{i,k} &= \begin{cases} a_{-i+k} & (k = i-\alpha, i-\alpha+1, \ldots, i+\alpha-1, i+\alpha), \\ 0 & (\text{otherwise}), \end{cases} \\ a^*_{i,k} &= -a_{k,i}, \\ \tilde{b}_{j,k} &= \begin{cases} b_{-j+k} & (k = j-\beta, j-\beta+1, \ldots, j+\beta-1, j+\beta), \\ 0 & (\text{otherwise}), \end{cases} \\ b^*_{j,k} &= -b_{k,j}.\end{aligned}$$

For $U_{i,j},\ V_{1,i,j}$ and $V_{2,i,j}$, we define a boundary term operator $\mu_{(\partial\Omega,\delta_\xi,\delta_\eta,x_\xi,x_\eta,y_\xi,y_\eta)}(\{U_{i,j}\},\{V_{1,i,j}\},\{V_{2,i,j}\})$ by

$$\begin{aligned}\mu_{(\partial\Omega,\delta_\xi,\delta_\eta,x_\xi,x_\eta,y_\xi,y_\eta)}(\{U_{i,j}\},\{V_{1,i,j}\},\{V_{2,i,j}\}) := &\sum_{j=0}^{M}\sum_{i=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}(y_\eta)_{i,j}\tilde{a}_{i,k}V_{1,k,j} - w_{i,j}^{-1}(x_\eta)_{i,j}\tilde{a}_{i,k}V_{2,k,j}\Big)\\
&+\sum_{j=0}^{M}\sum_{i=0}^{\alpha-1}\sum_{k=-\alpha}^{-1} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}(y_\eta)_{i,j}\tilde{a}_{i,k}V_{1,k,j} - w_{i,j}^{-1}(x_\eta)_{i,j}\tilde{a}_{i,k}V_{2,k,j}\Big)\\
&+\sum_{i=0}^{N}\sum_{j=M-\beta+1}^{M}\sum_{k=M+1}^{M+\beta} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}(x_\xi)_{i,j}\tilde{b}_{j,k}V_{2,i,k} - w_{i,j}^{-1}(y_\xi)_{i,j}\tilde{b}_{j,k}V_{1,i,k}\Big)\\
&+\sum_{i=0}^{N}\sum_{j=0}^{\beta-1}\sum_{k=-\beta}^{-1} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}(x_\xi)_{i,j}\tilde{b}_{j,k}V_{2,i,k} - w_{i,j}^{-1}(y_\xi)_{i,j}\tilde{b}_{j,k}V_{1,i,k}\Big)\\
&+\sum_{j=0}^{M}\sum_{i=N-\alpha+1}^{N}\sum_{k=N+1}^{N+\alpha} w_{i,j}U_{k,j}\Big(w_{i,j}^{-1}(y_\eta)_{k,j}\tilde{a}^*_{i,k}V_{1,i,j} - w_{i,j}^{-1}(x_\eta)_{k,j}\tilde{a}^*_{i,k}V_{2,i,j}\Big)\\
&+\sum_{j=0}^{M}\sum_{i=0}^{\alpha-1}\sum_{k=-\alpha}^{-1} w_{i,j}U_{k,j}\Big(w_{i,j}^{-1}(y_\eta)_{k,j}\tilde{a}^*_{i,k}V_{1,i,j} - w_{i,j}^{-1}(x_\eta)_{k,j}\tilde{a}^*_{i,k}V_{2,i,j}\Big)\\
&+\sum_{i=0}^{N}\sum_{j=M-\beta+1}^{M}\sum_{k=M+1}^{M+\beta} w_{i,j}U_{i,k}\Big(w_{i,j}^{-1}(x_\xi)_{i,k}\tilde{b}^*_{j,k}V_{2,i,j} - w_{i,j}^{-1}(y_\xi)_{i,k}\tilde{b}^*_{j,k}V_{1,i,j}\Big)\\
&+\sum_{i=0}^{N}\sum_{j=0}^{\beta-1}\sum_{k=-\beta}^{-1} w_{i,j}U_{i,k}\Big(w_{i,j}^{-1}(x_\xi)_{i,k}\tilde{b}^*_{j,k}V_{2,i,j} - w_{i,j}^{-1}(y_\xi)_{i,k}\tilde{b}^*_{j,k}V_{1,i,j}\Big).\end{aligned}$$

When $U_{i,j},\ V_{1,i,j}$ and $V_{2,i,j}$ approximate functions $u,\ v_1$ and v_2, respectively, this value approximates the boundary term (61) in the Gauss theorem.

We can now state the discrete Gauss theorem.

Lemma 19. *Let δ_ξ and δ_η be finite difference operators in the ξ and η directions, respectively. Let $U_{i,j},\ V_{1,i,j}$ and $V_{2,i,j}$ satisfy*

$$\mu_{(\partial\Omega,\delta_\xi,\delta_\eta,x_\xi,x_\eta,y_\xi,y_\eta)}(\{U_{i,j}\},\{V_{1,i,j}\},\{V_{2,i,j}\}) = 0.$$

Then

$$\begin{aligned}&\sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}\Big((y_\eta)_{i,j}\delta_\xi - (y_\xi)_{i,j}\delta_\eta\Big)V_{1,i,j} + w_{i,j}^{-1}\Big((x_\xi)_{i,j}\delta_\eta - (x_\eta)_{i,j}\delta_\xi\Big)V_{2,i,j}\Big)\\
&= -\sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}\Big(V_{1,i,j}w_{i,j}^{-1}\Big(\delta_\xi^*\Big((y_\eta)_{i,j}U_{i,j}\Big) - \delta_\eta^*\Big((y_\xi)_{i,j}U_{i,j}\Big)\Big) + V_{2,i,j}w_{i,j}^{-1}\Big(\delta_\eta^*\Big((x_\xi)_{i,j}U_{i,j}\Big) - \delta_\xi^*\Big((x_\eta)_{i,j}U_{i,j}\Big)\Big)\Big).\end{aligned} \tag{65}$$

Proof. The proof is the same as Lemma 17. Application of the summation by parts in the ξ and η directions gives

$$\begin{aligned}&\sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}\Big((y_\eta)_{i,j}\delta_\xi - (y_\xi)_{i,j}\delta_\eta\Big)V_{1,i,j} + w_{i,j}^{-1}\Big((x_\xi)_{i,j}\delta_\eta - (x_\eta)_{i,j}\delta_\xi\Big)V_{i,j}\Big)\\
&= \sum_{j=0}^{M}\sum_{i=0}^{N}\sum_{k=0}^{N} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}(y_\eta)_{i,j}\tilde{a}_{i,k}V_{1,k,j} - w_{i,j}^{-1}(x_\eta)_{i,j}\tilde{a}_{i,k}V_{2,k,j}\Big) + (\text{boundary term corresponding to } \delta_\xi)\\
&\quad+\sum_{i=0}^{N}\sum_{j=0}^{M}\sum_{k=0}^{M} w_{i,j}U_{i,j}\Big(w_{i,j}^{-1}(x_\xi)_{i,j}\tilde{b}_{j,k}V_{2,i,k} - w_{i,j}^{-1}(y_\xi)_{i,j}\tilde{b}_{j,k}V_{1,i,k}\Big) + (\text{boundary term corresponding to } \delta_\eta)\\
&= -\sum_{j=0}^{M}\sum_{k=0}^{N}\sum_{i=0}^{N} w_{k,j}U_{k,j}\Big(w_{k,j}^{-1}(y_\eta)_{k,j}\tilde{a}^*_{i,k}V_{1,i,j} - w_{k,j}^{-1}(x_\eta)_{k,j}\tilde{a}^*_{i,k}V_{2,i,j}\Big) + (\text{boundary term corresponding to } \delta_\xi)\\
&\quad-\sum_{i=0}^{N}\sum_{k=0}^{M}\sum_{j=0}^{M} w_{i,k}U_{i,k}\Big(w_{i,k}^{-1}(x_\xi)_{i,k}\tilde{b}^*_{j,k}V_{2,i,j} - w_{i,k}^{-1}(y_\xi)_{i,k}\tilde{b}^*_{j,k}V_{1,i,j}\Big) + (\text{boundary term corresponding to } \delta_\eta)\\
&= -\sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}\Big(V_{1,i,j}w_{i,j}^{-1}\Big(\delta_\xi^*\Big((y_\eta)_{i,j}U_{i,j}\Big) - \delta_\eta^*\Big((y_\xi)_{i,j}U_{i,j}\Big)\Big) - V_{2,i,j}w_{i,j}^{-1}\Big(\delta_\eta^*\Big((x_\xi)_{i,j}U_{i,j}\Big) - \delta_\xi^*\Big((x_\eta)_{i,j}U_{i,j}\Big)\Big)\Big)\\
&\quad+\Big(\text{boundary term corresponding to } \delta_\xi,\ \delta_\xi^*,\ \delta_\eta,\ \delta_\eta^*\Big).\end{aligned}$$

The straightforward calculation shows that the boundary term equals $\mu_{(\partial\Omega,\delta_\xi,\delta_\eta,x_\xi,x_\eta,y_\xi,y_\eta)}(\{U_{i,j}\},\{V_{1,i,j}\},\{V_{2,i,j}\})$. Therefore,

$$= -\sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}\left(V_{1,i,j}w_{i,j}^{-1}\left(\delta_\xi^*\left((y_\eta)_{i,j}U_{i,j}\right)-\delta_\eta^*\left((y_\xi)_{i,j}U_{i,j}\right)\right)-V_{2,i,j}w_{i,j}^{-1}\left(\delta_\eta^*\left((x_\xi)_{i,j}U_{i,j}\right)-\delta_\xi^*\left((x_\eta)_{i,j}U_{i,j}\right)\right)\right). \qquad \square$$

4.4. Definition of the discrete variational derivative

In this section, we define the discrete variational derivative on two-dimensional nonuniform meshes. Similar to one-dimensional case, the discrete variational derivative is defined so that it approximates the transformed variational derivative

$$\left(\frac{\delta G}{\delta u}\right)_{\mathrm{cs}} = \frac{\partial G}{\partial u} - \left(J^{-1}\left(\frac{\partial}{\partial\xi}\left(\frac{\partial y}{\partial\eta}\frac{\partial G}{\partial u_x}\right)-\frac{\partial}{\partial\eta}\left(\frac{\partial y}{\partial\xi}\frac{\partial G}{\partial u_x}\right)\right)+J^{-1}\left(\frac{\partial}{\partial\eta}\left(\frac{\partial x}{\partial\xi}\frac{\partial G}{\partial u_y}\right)-\frac{\partial}{\partial\xi}\left(\frac{\partial x}{\partial\eta}\frac{\partial G}{\partial u_y}\right)\right)\right).$$

We assume that the energy functional $G(u,u_x,u_y)$ is given in the next form:

$$G(u,u_x,u_y) = \sum_{l=1}^{K} f_l(u)g_l(u_x)h_l(u_y), \tag{66}$$

where f_l's, g_l's and h_l's are differentiable functions. We define the discrete energy functional $G_{\mathrm{d}}(\vec{U}^{(n)})_{i,j}$ by

$$G_{\mathrm{d}}(\vec{U}^{(n)})_{i,j} = \sum_{l=1}^{K} f_l\left(U_{i,j}^{(n)}\right)\left(\frac{1}{M_l}\sum_{m_l=1}^{M_l} g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)\right.$$
$$\left.\times h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)\right) \tag{67}$$

and the discrete total energy $H^{(n)}$ by

$$H^{(n)} = \sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}G_{\mathrm{d}}(\vec{U}^{(n)})_{i,j}. \tag{68}$$

Definition 5. The discrete variational derivative of $G_{\mathrm{d}}(\vec{U}^{(n)})_{i,j}$ is defined by

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j} = \sum_{l=1}^{K}\frac{1}{M_l}\sum_{m=1}^{M_l}\left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,i,j} - w_{i,j}^{-1}\left(\delta_{\xi,l,m}^*\left((y_\eta)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right)\right.\right.$$
$$\left.-\delta_{\eta,l,m}^*\left((y_\xi)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right)\right) - w_{i,j}^{-1}\left(\delta_{\eta,l,m}^*\left((x_\xi)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right)\right.$$
$$\left.\left.-\delta_{\xi,l,m}^*\left((x_\eta)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right)\right)\right\}, \tag{69}$$

where

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,i,j} = \frac{1}{6}\left(\frac{\mathrm{d}f_l}{\mathrm{d}(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{m,i,j}\left(2g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)}\right)\right.$$
$$h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)}\right)+g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)}\right)$$
$$h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)+g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)$$
$$h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)}\right)+2g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)$$
$$\left.h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)\right), \tag{70}$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j} = \frac{1}{6}\Big(2f_l\left(U_j^{(n+1)}\right)h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)}\right)$$
$$+f_l\left(U_j^{(n+1)}\right)h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)$$
$$+f_l\left(U_j^{(n)}\right)h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)}\right)$$
$$+2f_l(U_j^{(n)})h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)\Big)\left(\frac{\mathrm{d}g_l}{\mathrm{d}\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{m,i,j}, \tag{71}$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j} = \frac{1}{6}\Big(2f_l\left(U_j^{(n+1)}\right)g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)}\right)$$
$$+f_l\left(U_j^{(n+1)}\right)g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)$$
$$+f_l\left(U_j^{(n)}\right)g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)}\right)$$
$$+2f_l\left(U_j^{(n)}\right)g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)\Big)\left(\frac{\mathrm{d}h_l}{\mathrm{d}\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{m,i,j}, \tag{72}$$

$$\left(\frac{\mathrm{d}f_l}{\mathrm{d}(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{m,i,j} := \begin{cases} \frac{f_l\left(U_{i,j}^{(n+1)}\right) - f_l\left(U_{i,j}^{(n)}\right)}{U_{i,j}^{(n+1)} - U_{i,j}^{(n)}} & \left(U_{i,j}^{(n+1)} \neq U_{i,j}^{(n)}\right), \\ \frac{\mathrm{d}f_l}{\mathrm{d}U}\left(U_{i,j}^{(n)}\right) & (\text{otherwise}), \end{cases} \tag{73}$$

$$\left(\frac{\mathrm{d}g_l}{\mathrm{d}\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{m,i,j} := \begin{cases} \frac{g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)}\right) - g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)}{\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)} - \left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}} & (\text{if the denominator} \neq 0), \\ \frac{\mathrm{d}g_l}{\mathrm{d}U_x}\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m} - w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right) & (\text{otherwise}), \end{cases} \tag{74}$$

$$\left(\frac{\mathrm{d}h_l}{\mathrm{d}\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{m,i,j} := \begin{cases} \frac{h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)}\right) - h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)}{\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)} - \left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}} & (\text{if the denominator} \neq 0), \\ \frac{\mathrm{d}h_l}{\mathrm{d}U_y}\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m} - w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right) & (\text{otherwise}). \end{cases} \tag{75}$$

The discrete variational derivative is carefully defined again, which provides the variational structure:

Lemma 20. *Suppose the condition*

$$\mu_{(\partial\Omega,\delta_{\xi,l,m},\delta_{\eta,l,m},(x_\xi)_{l,m,i,j},(x_\eta)_{l,m,i,j},(y_\xi)_{l,m,i,j},(y_\eta)_{l,m,i,j})}\left(\left\{\frac{U_{i,j}^{(n+1)} - U_{i,j}^{(n)}}{\Delta t}\right\}, \left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right\}, \left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right\}\right) = 0 \tag{76}$$

is satisfied for each l and m. Then

$$\frac{1}{\Delta t}\left(H^{(n+1)} - H^{(n)}\right) = \sum_{i=0}^{N}\sum_{j=0}^{M} w_{i,j}\left(\frac{U_{i,j}^{(n+1)} - U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}. \tag{77}$$

Proof. From (70)–(72) we have

$$\frac{1}{\Delta t}\left(H^{(n+1)}-H^{(n)}\right)=\frac{1}{\Delta t}\sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{l=1}^{K}\frac{w_{i,j}}{M_l}\sum_{m_l=1}^{M_l}\left(f_l\left(U_{i,j}^{(n+1)}\right)\left(g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n+1)}\right)\right.\right.$$
$$h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n+1)}\right)\Big)$$
$$-f_l\left(U_{i,j}^{(n)}\right)\left(g_l\left(\left(w_{i,j}^{-1}(y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-w_{i,j}^{-1}(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)U_{i,j}^{(n)}\right)\right.$$
$$\left.\left.h_l\left(\left(w_{i,j}^{-1}(x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-w_{i,j}^{-1}(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)U_{i,j}^{(n)}\right)\right)\right)$$
$$=\sum_{i=0}^{N}\sum_{j=0}^{M}\sum_{l=1}^{K}\frac{w_{i,j}}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\partial G_{\rm d}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,i,j}\right.$$
$$+w_{i,j}^{-1}\left((y_\eta)_{l,m,i,j}\delta_{\xi,l,m}-(y_\xi)_{l,m,i,j}\delta_{\eta,l,m}\right)\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}$$
$$\left.+w_{i,j}^{-1}\left((x_\xi)_{l,m,i,j}\delta_{\eta,l,m}-(x_\eta)_{l,m,i,j}\delta_{\xi,l,m}\right)\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right).$$

Applying Lemma 19, we obtain

$$=\sum_{i=0}^{N}\sum_{j=0}^{M}\sum_{l=1}^{K}\frac{w_{i,j}}{M_l}\sum_{m=1}^{M_l}\left[\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\partial G_{\rm d}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,i,j}-w_{i,j}^{-1}\left\{\delta^*_{\xi,l,m}\left((y_\eta)_{l,m,i,j}\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right)\right.\right.$$
$$\left.-\delta^*_{\eta,l,m}\left((y_\xi)_{l,m,i,j}\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right)\right\}\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)-w_{i,j}^{-1}\left\{\delta^*_{\eta,l,m}\left((x_\xi)_{l,m,i,j}\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right)\right.$$
$$\left.\left.-\delta^*_{\xi,l,m}\left((x_\eta)_{l,m,i,j}\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right)\right\}\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\right]=\sum_{j=0}^{N}w_{i,j}\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}. \qquad \square$$

4.5. Design of schemes for the dissipative equations

We define the scheme for the dissipative equation (44) by

$$\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}=-\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j} \tag{78a}$$

if $s=0$, and by

$$\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}=w_{i,j}^{-1}\delta^*_\xi\left((y_\eta)_{i,j}\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)\right)\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)$$
$$-w_{i,j}^{-1}\delta^*_\eta\left((y_\xi)_{i,j}\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)\right)\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)$$
$$+w_{i,j}^{-1}\delta^*_\eta\left((x_\xi)_{i,j}\left(w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)$$
$$-w_{i,j}^{-1}\delta^*_\xi\left((x_\eta)_{i,j}\left(w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right) \tag{78b}$$

if $s=1$.

Theorem 21. *Let $w_{i,j}$'s be positive. Let $U_{i,j}^{(n)}$ be a numerical solution of the scheme (78a) or (78b) under the boundary condition that satisfies the assumption of Lemma 20 . Suppose also that*

$$\mu_{(\partial\Omega,\delta_\xi,\delta_\eta,(x_\xi)_{i,j},(x_\eta)_{i,j},(y_\xi)_{i,j},(y_\eta)_{i,j})}\left(\left\{\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\},\left\{w_{k,j}^{-1}\left((y_\eta)_{k,j}\delta_\xi-(y_\xi)_{k,j}\delta_\eta\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\},\right.$$
$$\left.\left\{w_{k,j}^{-1}\left((x_\xi)_{k,j}\delta_\eta-(x_\eta)_{k,j}\delta_\xi\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\}\right)=0 \tag{79}$$

if $s=1$. *Then*

$$\frac{1}{\Delta t}\left(H^{(n+1)}-H^{(n)}\right)\leqslant 0. \tag{80}$$

Proof. This theorem is obtained in almost the same way as Theorem 15. By Lemma 20, we have

$$\frac{1}{\Delta t}\left(H^{(n+1)}-H^{(n)}\right)=\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}. \tag{81}$$

In the case of $s=0$, substituting scheme (78a) yields

$$(81)=-\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)^2\leqslant 0.$$

In the case of $s=1$, substituting scheme (78b) and applying Lemma 19 yield

$$\begin{aligned}(81)=&-\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\left(w_{i,j}^{-1}\delta_\xi^*\left((y_\eta)_{i,j}\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right.\\
&-w_{i,j}^{-1}\delta_\eta^*\left((y_\xi)_{i,j}\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\\
&+w_{i,j}^{-1}\delta_\eta^*\left((x_\xi)_{i,j}\left(w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\\
&\left.-w_{i,j}^{-1}\delta_\xi^*\left((x_\eta)_{i,j}\left(w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\\
=&-\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)^2\right.\\
&\left.+\left(w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)^2\right)\leqslant 0.\qquad\square\end{aligned}$$

4.6. Design of schemes for the conservative equations

We define the scheme for the conservative equation (47) by

$$\begin{aligned}\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}=\frac{1}{2}\Bigg\{&\left(w_{i,j}^{-1}((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta)+w_{i,j}^{-1}((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi)\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\\
&+w_{i,j}^{-1}\left(\delta_\xi\left((y_\eta)_{i,j}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)-\delta_\eta\left((y_\xi)_{i,j}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_\eta\left((x_\xi)_{i,j}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)-\delta_\xi\left((x_\eta)_{i,j}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\Bigg\},\end{aligned} \tag{82}$$

where δ_ξ and δ_η are the central difference operators in the ξ and the η directions, respectively.

Theorem 22. *Let $U_{i,j}^{(n)}$ be a numerical solution of scheme (82) under the boundary condition that satisfies the assumption of Lemma 20 and*

$$\mu_{(\partial\Omega,\delta_c,\delta_c,(x_\xi)_{i,j},(x_\eta)_{i,j},(y_\xi)_{i,j},(y_\eta)_{i,j})}\left(\left\{\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\},\left\{\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\},\left\{\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\}\right)=0. \tag{83}$$

Then

$$\frac{1}{\Delta t}(H^{(n+1)}-H^{(n)})=0. \tag{84}$$

Proof. This theorem is obtained in almost the same way as Theorem 16. Applying Lemma 20 we have

$$\frac{1}{\Delta t}\left(H^{(n+1)}-H^{(n)}\right)=\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t}\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}.$$

Substituting scheme (82) yields

$$\begin{aligned}&=\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\left\{\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)+w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right.\\&+w_{i,j}^{-1}\left(\delta_\xi\left((y_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)-\delta_\eta\left((y_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)+w_{i,j}^{-1}\left(\delta_\eta\left((x_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right.\\&\left.\left.-\delta_\xi\left((x_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\right\}.\end{aligned}$$

Applying Lemma 19 gives

$$\begin{aligned}&=-\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\left\{w_{i,j}^{-1}\left(\delta_\eta^*\left((x_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)-\delta_\xi^*\left((x_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\right.\\&+w_{i,j}^{-1}\left(\delta_\xi^*\left((y_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)-\delta_\eta^*\left((y_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi^*-(y_\xi)_{i,j}\delta_\eta^*\right)\right.\\&\left.\left.+w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta^*-(x_\eta)_{i,j}\delta_\xi^*\right)\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\}.\end{aligned}$$

Since $\delta_\xi=\delta_c=\delta_c^*=\delta_\xi^*$ and $\delta_\eta=\delta_c=\delta_c^*=\delta_\eta^*$, it follows that

$$\begin{aligned}\frac{1}{\Delta t}(H^{(n+1)}-H^{(n)})=&\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\left\{\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)\right.\right.\\&\left.+w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}+w_{i,j}^{-1}\left(\delta_\xi\left((y_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right.\\&\left.\left.-\delta_\eta\left((y_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)+w_{i,j}^{-1}\left(\delta_\eta\left((x_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)-\delta_\xi\left((x_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\right\}\\=&-\frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{M}w_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\left\{w_{i,j}^{-1}\left(\delta_\eta\left((x_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right.\right.\\&\left.-\delta_\xi\left((x_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)+w_{i,j}^{-1}\left(\delta_\xi\left((y_\eta)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right.\\&\left.\left.-\delta_\eta\left((y_\xi)_{i,j}\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\right)\left(w_{i,j}^{-1}\left((y_\eta)_{i,j}\delta_\xi-(y_\xi)_{i,j}\delta_\eta\right)+w_{i,j}^{-1}\left((x_\xi)_{i,j}\delta_\eta-(x_\eta)_{i,j}\delta_\xi\right)\right)\left(\frac{\delta G_d}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right\},\end{aligned}$$

and hence this equals 0. □

5. An example of the two-dimensional case

As an example of the two-dimensional case, we derive a dissipative scheme and show a numerical result for the Cahn–Hilliard equation

$$\frac{\partial u}{\partial t} = \Delta \frac{\delta G}{\delta u}, \quad G(u, u_x, u_y) = \frac{p}{2}u^2 + \frac{r}{4}u^4 - \frac{q}{2}\left(\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2\right). \tag{85}$$

5.1. An energy dissipative scheme for the Cahn–Hilliard equation

We first define the discrete energy functional for this equation. The energy functional $G(u, u_x, u_y)$ is written in the form of (66) with $K = 3$ and

$$\begin{aligned}
&f_1(u) = \frac{p}{2}u^2 + \frac{r}{4}u^4, \quad f_2(u) = 1, \quad f_3(u) = 1, \\
&g_1(u_x) = 1, \quad g_2(u_x) = -\frac{q}{2}u_x^2, \quad g_3(u_x) = 1, \\
&h_1(u_y) = 1, \quad h_2(u_y) = 1, \quad h_3(u_y) = -\frac{q}{2}u_y^2.
\end{aligned}$$

We introduce the discrete energy functional so that it corresponds to these. On the given mesh, we introduce the weights by

$$\begin{aligned}
&w_{i,j} = (x_{\xi,c})_{i,j}(y_{\eta,c})_{i,j} - (x_{\eta,c})_{i,j}(y_{\xi,c})_{i,j}, \\
&(x_{\xi,c})_{i,j} = \frac{x(i+1,j) - x(i-1,j)}{2}, \quad (y_{\xi,c})_{i,j} = \frac{y(i+1,j) - y(i-1,j)}{2}, \\
&(x_{\eta,c})_{i,j} = \frac{x(i,j+1) - x(i,j-1)}{2}, \quad (y_{\eta,c})_{i,j} = \frac{y(i,j+1) - y(i,j-1)}{2}.
\end{aligned}$$

The following difference operators are used for the discretization:

$$\delta_{\xi,+}U_{i,j} = U_{i+1,j} - U_{i,j}, \quad \delta_{\xi,-}U_{i,j} = U_{i,j} - U_{i-1,j}, \quad \delta_{\eta,+}U_{i,j} = U_{i,j+1} - U_{i,j}, \quad \delta_{\eta,-}U_{i,j} = U_{i,j} - U_{i,j-1}.$$

For $l = 2,\ M_2 = 4$ is set and g_2 is approximated by

$$\begin{aligned}
g_2(u_x) = -\frac{q}{2}u_x^2 \simeq -\frac{1}{M_2}\frac{q}{2}\Bigg(&\left(w_{i,j}^{-1}((y_{\eta,c})_{i,j}\delta_{\xi,+} - (y_{\xi,c})_{i,j}\delta_{\eta,+})U_{i,j}^{(n)}\right)^2 + \left(w_{i,j}^{-1}((y_{\eta,c})_{i,j}\delta_{\xi,+} - (y_{\xi,c})_{i,j}\delta_{\eta,-})U_{i,j}^{(n)}\right)^2 \\
&+\left(w_{i,j}^{-1}((y_{\eta,c})_{i,j}\delta_{\xi,-} - (y_{\xi,c})_{i,j}\delta_{\eta,+})U_{i,j}^{(n)}\right)^2 + \left(w_{i,j}^{-1}((y_{\eta,c})_{i,j}\delta_{\xi,-} - (y_{\xi,c})_{i,j}\delta_{\eta,-})U_{i,j}^{(n)}\right)^2\Bigg),
\end{aligned}$$

which gives

$$\begin{aligned}
&(y_\xi)_{2,1,i,j} = (y_\xi)_{2,2,i,j} = (y_\xi)_{2,3,i,j} = (y_\xi)_{2,4,i,j} = (y_{\xi,c})_{i,j}, \\
&(y_\eta)_{2,1,i,j} = (y_\eta)_{2,2,i,j} = (y_\eta)_{2,3,i,j} = (y_\eta)_{2,4,i,j} = (y_{\eta,c})_{i,j}, \\
&\delta_{\xi,2,1} = \delta_{\xi,2,2} = \delta_{\xi,+}, \quad \delta_{\xi,2,3} = \delta_{\xi,2,4} = \delta_{\xi,-}, \quad \delta_{\eta,2,1} = \delta_{\eta,2,3} = \delta_{\eta,+}, \quad \delta_{\eta,2,2} = \delta_{\eta,2,4} = \delta_{\eta,-}.
\end{aligned}$$

Similarly, we set $M_3 = 4$ and approximate h_3 by

$$\begin{aligned}
h_3(u_y) = -\frac{q}{2}u_y^2 \simeq -\frac{1}{M_3}\frac{q}{2}\Bigg(&\left(w_{i,j}^{-1}((x_{\xi,c})_{i,j}\delta_{\eta,+} - (x_{\eta,c})_{i,j}\delta_{\xi,+})U_{i,j}^{(n)}\right)^2 + \left(w_{i,j}^{-1}((x_{\xi,c})_{i,j}\delta_{\eta,+} - (x_{\eta,c})_{i,j}\delta_{\xi,-})U_{i,j}^{(n)}\right)^2 \\
&+\left(w_{i,j}^{-1}((x_{\xi,c})_{i,j}\delta_{\eta,-} - (x_{\eta,c})_{i,j}\delta_{\xi,+})U_{i,j}^{(n)}\right)^2 + \left(w_{i,j}^{-1}((x_{\xi,c})_{i,j}\delta_{\eta,-} - (x_{\eta,c})_{i,j}\delta_{\xi,-})U_{i,j}^{(n)}\right)^2\Bigg),
\end{aligned}$$

which gives

$$\begin{aligned}
&(x_\xi)_{3,1,i,j} = (x_\xi)_{3,2,i,j} = (x_\xi)_{3,3,i,j} = (x_\xi)_{3,4,i,j} = (x_{\xi,c})_{i,j}, \\
&(x_\eta)_{3,1,i,j} = (x_\eta)_{3,2,i,j} = (x_\eta)_{3,3,i,j} = (x_\eta)_{3,4,i,j} = (x_{\eta,c})_{i,j}, \\
&\delta_{\xi,3,1} = \delta_{\xi,3,3} = \delta_{\xi,+}, \quad \delta_{\xi,3,2} = \delta_{\xi,3,4} = \delta_{\xi,-}, \quad \delta_{\eta,3,1} = \delta_{\eta,3,2} = \delta_{\eta,+}, \quad \delta_{\eta,3,3} = \delta_{\eta,3,4} = \delta_{\eta,-}.
\end{aligned}$$

From the above, the discrete energy functional is defined by

$$\begin{aligned}G_{\mathrm{d}}(\vec{U}^{(n)})_{i,j} = &\frac{p}{2}\left(U^{(n)}_{i,j}\right)^2 + \frac{r}{4}\left(U^{(n)}_{i,j}\right)^4 - \frac{1}{M_2}\frac{q}{2}\Bigg(\left(w^{-1}_{i,j}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}\right)U^{(n)}_{i,j}\right)^2 \\ &+\left(w^{-1}_{i,j}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}\right)U^{(n)}_{i,j}\right)^2 + \left(w^{-1}_{i,j}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+})U^{(n)}_{i,j}\right)^2 \\ &+\left(w^{-1}_{i,j}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})U^{(n)}_{i,j}\right)^2\Bigg) - \frac{1}{M_3}\frac{q}{2}\Bigg(\left(w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})U^{(n)}_{i,j}\right)^2 \\ &+\left(w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})U^{(n)}_{i,j}\right)^2 + \left(w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})U^{(n)}_{i,j}\right)^2 \\ &+\left(w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})U^{(n)}_{i,j}\right)^2\Bigg).\end{aligned}$$

Next, we define the discrete variational derivative by (69). For $l = 1$, we set $M_1 = 1$ and obtain

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{1,1,i,j} = \frac{p}{2}\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right) + \frac{r}{4}\left(\left(U^{(n+1)}_{i,j}\right)^3 + \left(U^{(n+1)}_{i,j}\right)^2 U^{(n)}_{i,j} + U^{(n+1)}_{i,j}\left(U^{(n)}_{i,j}\right)^2 + \left(U^{(n)}_{i,j}\right)^3\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)}_x, \vec{U}^{(n)}_x)}\right)_{1,1,i,j} = \left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_y, \vec{U}^{(n)}_y\right)}\right)_{1,1,i,j} = 0.$$

For $l = 2$, we have already set $M_2 = 4$ and obtain

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_x, \vec{U}^{(n)}_x\right)}\right)_{2,1,i,j} = -\frac{q}{2}w^{-1}_{i,j}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}\right)\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_x, \vec{U}^{(n)}_x\right)}\right)_{2,2,i,j} = -\frac{q}{2}w^{-1}_{i,j}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}\right)\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_x, \vec{U}^{(n)}_x\right)}\right)_{2,3,i,j} = -\frac{q}{2}w^{-1}_{i,j}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}\right)\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_x, \vec{U}^{(n)}_x\right)}\right)_{2,4,i,j} = -\frac{q}{2}w^{-1}_{i,j}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-} - (y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}\right)\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{2,m,i,j} = \left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_y, \vec{U}^{(n)}_y\right)}\right)_{2,m,i,j} = 0 \quad (m = 1,2,3,4).$$

In a similar manner, for $l = 3$ we have

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_y, \vec{U}^{(n)}_y\right)}\right)_{3,1,i,j} = -\frac{q}{2}w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_y, \vec{U}^{(n)}_y\right)}\right)_{3,2,i,j} = -\frac{q}{2}w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_y, \vec{U}^{(n)}_y\right)}\right)_{3,3,i,j} = -\frac{q}{2}w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_y, \vec{U}^{(n)}_y\right)}\right)_{3,4,i,j} = -\frac{q}{2}w^{-1}_{i,j}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-} - (x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\left(U^{(n+1)}_{i,j} + U^{(n)}_{i,j}\right),$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)}, \vec{U}^{(n)})}\right)_{3,m,i,j} = \left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}^{(n+1)}_x, \vec{U}^{(n)}_x\right)}\right)_{3,m,i,j} = 0 \quad (m = 1,2,3,4).$$

Using the above symbols, the discrete variational derivative is defined by

$$
\begin{aligned}
\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j} ={}& \sum_{l=1}^{3}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{\partial G_{\mathrm{d}}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,i,j} - w_{i,j}^{-1}\left(\delta^{*}_{\xi,l,m}\left((y_\eta)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right)\right.\right.\\
&\left.-\delta^{*}_{\eta,l,m}\left((y_\xi)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,i,j}\right)\right) - w_{i,j}^{-1}\left(\delta^{*}_{\eta,l,m}\left((x_\xi)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right)\right.\\
&\left.\left.-\delta^{*}_{\xi,l,m}\left((x_\eta)_{l,m,i,j}\left(\frac{\partial G_{\mathrm{d}}}{\partial\left(\vec{U}_y^{(n+1)},\vec{U}_y^{(n)}\right)}\right)_{l,m,i,j}\right)\right)\right) = \frac{p}{2}\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)+\frac{r}{4}\left(\left(U_{i,j}^{(n+1)}\right)^3\right.\\
&\left.+\left(U_{i,j}^{(n+1)}\right)^2U_{i,j}^{(n)}+U_{i,j}^{(n+1)}\left(U_{i,j}^{(n)}\right)^2+\left(U_{i,j}^{(n)}\right)^3\right)-\frac{q}{8}\left(w_{i,j}^{-1}\left(\delta_{\xi,-}\left((y_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}\left((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}\right)\right.\right.\right.\\
&\left.\left.\times\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)-\delta_{\eta,-}\left((y_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_{\xi,-}\left((y_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\\
&\left.-\delta_{\eta,+}\left((y_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_{\xi,+}\left((y_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\\
&\left.-\delta_{\eta,-}\left((y_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_{\xi,+}\left((y_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\\
&\left.\left.-\delta_{\eta,+}\left((y_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\right)\\
&-\frac{q}{8}\left(w_{i,j}^{-1}\left(\delta_{\eta,-}\left((x_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\right.\\
&\left.-\delta_{\xi,-}\left((x_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_{\eta,-}\left((x_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\\
&\left.-\delta_{\xi,+}\left((x_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,+}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_{\eta,+}\left((x_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\\
&\left.-\delta_{\xi,-}\left((x_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,+})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\\
&+w_{i,j}^{-1}\left(\delta_{\eta,+}\left((x_{\xi,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right.\\
&\left.\left.-\delta_{\xi,+}\left((x_{\eta,\mathrm{c}})_{i,j}w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\left(U_{i,j}^{(n+1)}+U_{i,j}^{(n)}\right)\right)\right)\right).
\end{aligned}
$$

The scheme is defined by (78b) with, for example, δ_ξ and δ_η being the backward differences $\delta_{\xi,-}$ and $\delta_{\eta,-}$:

$$
\begin{aligned}
\frac{U_{i,j}^{(n+1)}-U_{i,j}^{(n)}}{\Delta t} ={}& w_{i,j}^{-1}\delta_{\xi,+}\left((y_{\eta,\mathrm{c}})_{i,j}\left(w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\\
&-w_{i,j}^{-1}\delta_{\eta,+}\left((y_{\xi,\mathrm{c}})_{i,j}\left(w_{i,j}^{-1}((y_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-}-(y_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-})\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\\
&+w_{i,j}^{-1}\delta_{\eta,+}\left((x_{\xi,\mathrm{c}})_{i,j}\left(w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right)\\
&-w_{i,j}^{-1}\delta_{\xi,+}\left((x_{\eta,\mathrm{c}})_{i,j}\left(w_{i,j}^{-1}((x_{\xi,\mathrm{c}})_{i,j}\delta_{\eta,-}-(x_{\eta,\mathrm{c}})_{i,j}\delta_{\xi,-})\right)\left(\frac{\delta G_{\mathrm{d}}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{i,j}\right).
\end{aligned}
$$

5.2. Numerical example

We solved the Cahn–Hilliard equation on the annular domain Ω, as shown in Fig. 6, using the scheme derived in the previous section. The parameters of the equation were set to $p=-1,\ q=-0.001$ and $r=1$. The domain Ω is represented as

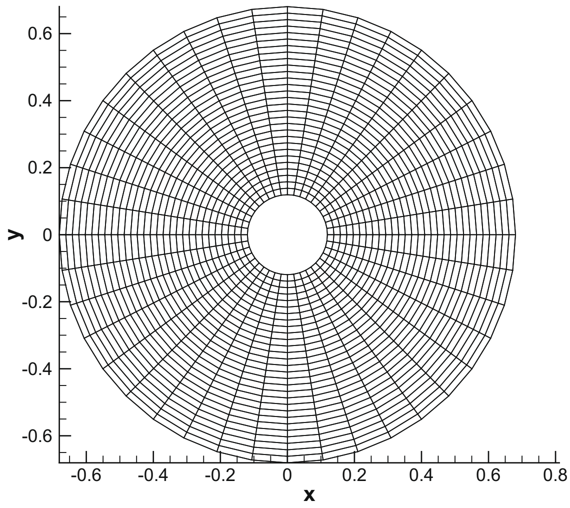


Fig. 6. The mesh used for the computation.

$\Omega = \{(x,y)|x = \rho\cos\theta,\ y = \rho\sin\theta,\ 0.1 \leqslant \rho \leqslant 0.7,\ 0 \leqslant \theta < 2\pi\}$ by the polar coordinate. We used the grid shown in Fig. 6, which is written as

$$x(\xi,\eta) = \rho(\xi)\cos(\theta(\eta)), \quad y(\xi,\eta) = \rho(\xi)\sin(\theta(\eta)), \quad \rho(\xi) = \frac{3}{5}\frac{\xi}{N} + \frac{1}{10}, \quad \theta(\eta) = \frac{2\pi\eta}{M+1} \tag{86}$$

in the computational space. The number of nodes are 30 in the ξ direction and 40 in the η direction. We set the periodic boundary condition in the η direction and

$$\frac{\partial u}{\partial \xi} = 0, \quad \frac{\partial}{\partial \xi}(\Delta u) = 0 \tag{87}$$

in the ξ direction. Under these conditions, the solution has the dissipation property. Additionally, the Cahn–Hilliard equation describes the phase separation and the solution u denotes the density of the materials. Under the above conditions, the total density is also conserved:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega u\,\mathrm{d}x\,\mathrm{d}y = 0.$$

The initial condition is set by

$$u(0,\xi,\eta) = 0.001\sin(10\pi(r(\xi) - 0.1)) + 0.001\sin(7\theta(\eta)). \tag{88}$$

As a naive method, it is natural to employ the implicit Euler method in time and the central difference that approximates the Laplace operator in the polar coordinate

$$\Delta = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \theta^2}.$$

Therefore, we compared our method with this naive method, using MINPACK to solve the nonlinear systems.

When the naive method was used, the scheme was unstable, even with $\Delta t = 10^{-7}$. This result is due to the fact that the naive method does not retain either the energy dissipation property or the conservation of the total density. Both the total energy $H^{(n)}$ and the total density $\sum_{i,j} w_{i,j} U_{i,j}^{(n)}$ diverge, as shown in Figs. 7 and 9.

On the other hand, our scheme is stable with $\Delta t = 10^{-3}$. Although the total computation time is approximately 1 h and 27 s with a 3.00 GHz Intel Core2 Duo CPU (only one core is used), this is improved to 1 min and 42 s when DF-SANE [6], which is a more modern quasi-Newton method, is applied. The time evolutions of the total energy and the total density in that case are shown in Figs. 8 and 10. The dissipation property of our scheme is confirmed by Fig. 8. Additionally, although the proof is omitted, the total density is preserved in our scheme, which is confirmed by Fig. 10. The numerical solutions at $t = 0.0, 0.05, 0.08, 0.12, 0.15, 0.75$ obtained using our scheme are shown in Figs. 11–16. The black and the white regions in the figures correspond to the regions where the values of u are almost -1 and 1, respectively. They represent the different phases and the total energy decreases when the phases coalesce. The coalescence of the black regions is observed from $t = 0.05$ to $t = 0.08$, while a decrease in the energy is observed simultaneously. A similar phenomena can also be observed from $t = 0.12$ to $t = 0.15$ and from $t = 0.15$ to $t = 0.75$.

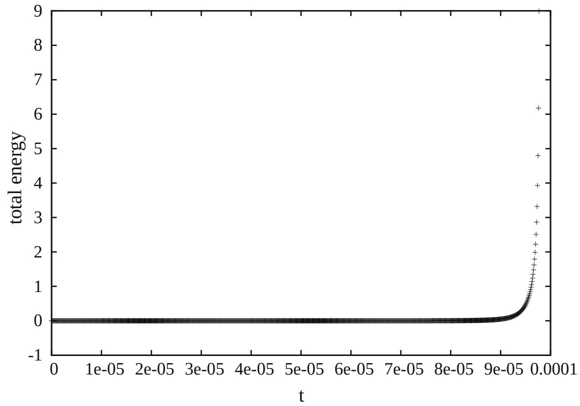


Fig. 7. Time evolution of the total energy of the numerical solution computed using the naive scheme.

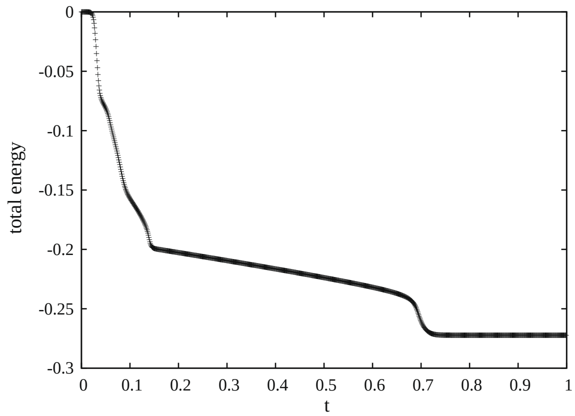


Fig. 8. Time evolution of the total energy of the numerical solution computed using our scheme.

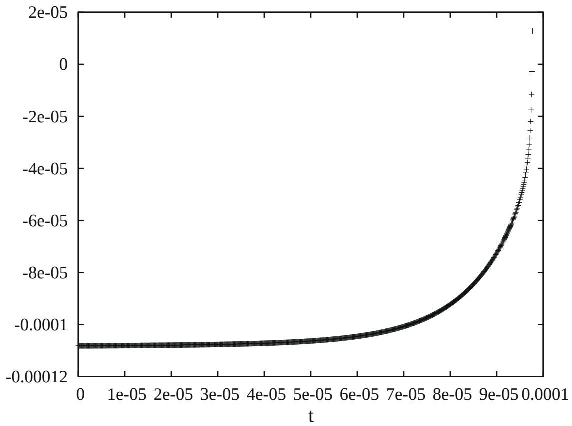


Fig. 9. Time evolution of the total density of the numerical solution computed using the naive scheme.

Moreover, our scheme works even when the initial condition is given as random numbers. Figs. 17–20 show the numerical results with such an initial condition, where the initial value at each point is given by a uniform random number in $[-0.05, 0.05]$. The dissipation property is again confirmed as shown in Fig. 21.

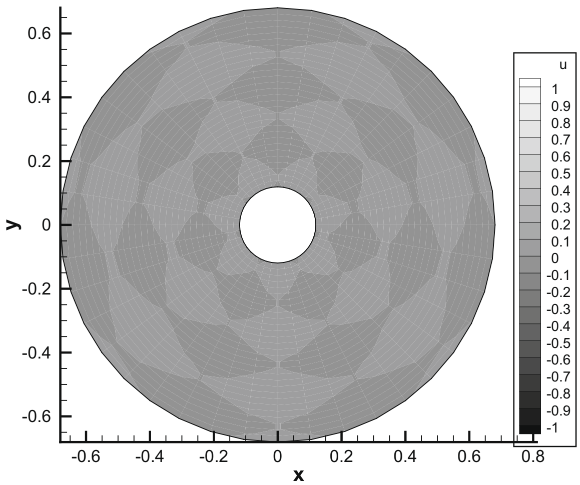
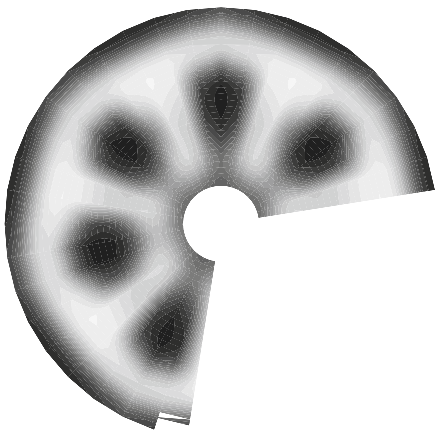
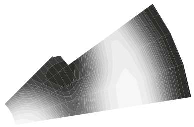
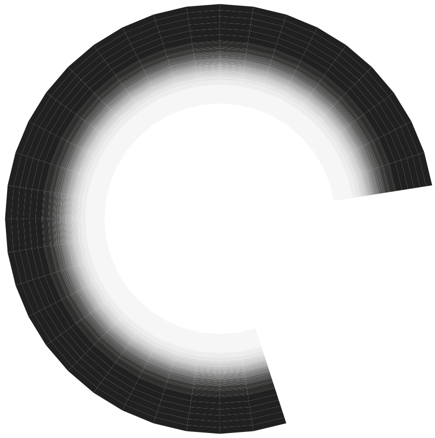
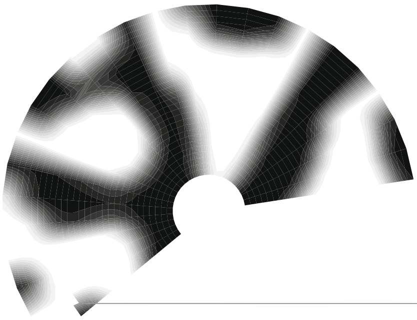


Fig. 11. The initial condition (88).









6. Dissipative/conservative schemes for complex valued equations

The discrete variational method has been extended to equations other than those of the form (3) or (5), which include complex valued equations and nonlinear wave equations [9,14,16]. Our extension can be also applied to such equations. As an example, we demonstrate application to one-dimensional complex valued equations. The extension to the two-dimensional case is obtained in the same way as described in Section 4. The proofs of the theorems are omitted below, but they are proved in similar ways to those shown in the previous sections. The original discrete variational method for such equations is shown in [16].

We consider the dissipative equations

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \bar{u}} \tag{89}$$

and the conservative equations

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \bar{u}}, \tag{90}$$

where u is a complex valued function and $\bar{u}$ denotes the complex conjugate. The dissipative equations include the Ginzburg–Landau equation

$$\frac{\partial u}{\partial t} = p\frac{\partial^2 u}{\partial x^2} + q|u|^2 u + ru,$$

where $p,\ q$ and r are real parameters, and the conservative equation is the nonlinear Schrödinger equation

$$\mathrm{i}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \gamma|u|^{p-1}u,$$

where γ is a real parameter. The variational derivatives are defined by

$$\frac{\delta G}{\delta u} = \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}, \quad \frac{\delta G}{\delta \bar{u}} = \frac{\partial G}{\partial \bar{u}} - \frac{\partial}{\partial x}\frac{\partial G}{\partial \bar{u}_x}.$$

The energy functional $G(u, u_x)$ is assumed to be of the following form:

$$G(u, u_x) = \sum_{l=1}^{K} f_l(u) g_l(u_x),$$

where $f_l(u)$ and $g_l(u_x)$ are read valued functions that satisfy

$$f_l(u) = f_l(\bar{u}), \quad g_l(u_x) = g_l(\bar{u}_x).$$

As is well-known [16], equations of the form (89) are dissipative.

Theorem 23. *Suppose that the boundary condition satisfies*

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \bar{u}_x}\frac{\partial \bar{u}}{\partial t}\right]_0^L = 0.$$

The solutions of (89) then have the dissipation property:

$$\frac{d}{dt}\int_0^L G(u, u_x)dx \leqslant 0.$$

Similarly, equations of the form (90) are conservative.

Theorem 24. *Suppose that the boundary condition satisfies*

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \bar{u}_x}\frac{\partial \bar{u}}{\partial t}\right]_0^L = 0.$$

The solutions of (90) then have the conservation property:

$$\frac{d}{dt}\int_0^L G(u, u_x)dx = 0.$$

6.1. Definition of the discrete variational derivative

We can introduce the discrete variational derivatives for these equations in a similar way to that in Section 2. We define the discrete energy functional by

$$G_{\rm d}(\vec{U})_j^{(n)} = \sum_{l=1}^{K} f_l\left(U_j^{(n)}\right)\left(\frac{1}{M_l}\sum_{m=1}^{M_l} g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right)\right)$$

and the discrete total energy $H^{(n)}$ by (29).

Definition 6. The discrete variational derivatives of $G_{\rm d}(\vec{U})_j^{(n)}$ are defined by

$$\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j := \sum_{l=1}^{K}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{\partial G_{\rm d}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,j} - w_j^{-1}\delta_{l,m}^{*}\left((x_\xi)_{l,m,j}^{-1}w_j\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right)\right),$$

$$\left(\frac{\partial G_{\rm d}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,j} := \left(\frac{f_l\left(U_j^{(n+1)}\right)-f_l\left(U_j^{(n)}\right)}{\left|U_j^{(n+1)}\right|^2-\left|U_j^{(n)}\right|^2}\right)\left(\overline{\frac{U_j^{(n+1)}+U_j^{(n)}}{2}}\right)\left(\frac{g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}\right)+g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right)}{2}\right),$$

$$\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j} := \left(\frac{f_l\left(U_j^{(n+1)}\right)+f_l(U_j^{(n)})}{2}\right)\left(\frac{g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}\right)-g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right)}{\left|(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}\right|^2-\left|(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right|^2}\right)\left(\overline{\frac{(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}+(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}}{2}}\right)$$

and

$$\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j := \sum_{l=1}^{K}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\left(\frac{\partial G_{\rm d}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,j} - w_j^{-1}\delta_{l,m}^{*}\left((x_\xi)_{l,m,j}^{-1}w_j\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right)\right),$$

$$\left(\frac{\partial G_{\rm d}}{\partial(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_{l,m,j} := \left(\frac{f_l\left(U_j^{(n+1)}\right)-f_l\left(U_j^{(n)}\right)}{\left|U_j^{(n+1)}\right|^2-\left|U_j^{(n)}\right|^2}\right)\left(\frac{U_j^{(n+1)}+U_j^{(n)}}{2}\right)\left(\frac{g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}\right)+g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right)}{2}\right),$$

$$\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j} := \left(\frac{f_l\left(U_j^{(n+1)}\right)+f_l(U_j^{(n)})}{2}\right)\left(\frac{g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}\right)-g_l\left((x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right)}{\left|(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}\right|^2-\left|(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}\right|^2}\right)\left(\frac{(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n+1)}+(x_\xi)_{l,m,j}^{-1}\delta_{l,m}U_j^{(n)}}{2}\right).$$

Lemma 25. *Suppose the boundary condition satisfies*

$$\sum_{l=1}^{K}\frac{1}{M_l}\sum_{m=1}^{M_l}\left(\mu_{(+,\delta_{l,m},(x_\xi)_{l,m,j}^{-1})}\left(\left\{\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right\},\left\{\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right\}\right)\right.$$
$$\left.+\mu_{(-,\delta_{l,m},(x_\xi)_{l,m,j}^{-1})}\left(\left\{\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right\},\left\{\left(\frac{\partial G_{\rm d}}{\partial\left(\vec{U}_x^{(n+1)},\vec{U}_x^{(n)}\right)}\right)_{l,m,j}\right\}\right)\right)+({\rm C.C.})=0$$

where (C.C.) denotes the complex conjugate of the other terms. Then

$$\frac{1}{\Delta t}(H^{(n+1)}-H^{(n)}) = \sum_{j=0}^{N} w_j\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right)\left(\frac{\delta G_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j + ({\rm C.C.}).$$

6.2. Design of schemes

We define the scheme for the dissipative equation of the form (89) by

$$\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right) = -\left(\frac{\delta\vec{G}_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \tag{91}$$

and by

$$\mathrm{i}\left(\frac{U_j^{(n+1)}-U_j^{(n)}}{\Delta t}\right) = -\left(\frac{\delta\vec{G}_{\rm d}}{\delta(\vec{U}^{(n+1)},\vec{U}^{(n)})}\right)_j \tag{92}$$

for the conservative equation of the form (90).

Theorem 26. *Let w_j's be positive. Let $U_j^{(n)}$ be a numerical solution of scheme (91) under the boundary condition that satisfies the assumption of Lemma 25. Then*

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

Theorem 27. *Let $U_j^{(n)}$ be a numerical solution of scheme (92) under the boundary condition that satisfies the assumption of Lemma 25. Then*

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

7. Concluding remarks

We have extended the discrete variational method to nonuniform meshes. Although we have considered one- and the two-dimensional cases for simplicity, conservative/dissipative schemes can also be derived for three-dimensional cases by transforming the differential operators to, for example,

$$\frac{\partial}{\partial x} = \frac{1}{J}\left(\left(\frac{\partial y}{\partial \eta}\frac{\partial z}{\partial \zeta} - \frac{\partial y}{\partial \zeta}\frac{\partial z}{\partial \eta}\right)\frac{\partial}{\partial \xi} + \left(\frac{\partial y}{\partial \zeta}\frac{\partial z}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial z}{\partial \zeta}\right)\frac{\partial}{\partial \eta} + \left(\frac{\partial y}{\partial \xi}\frac{\partial z}{\partial \eta} - \frac{\partial y}{\partial \eta}\frac{\partial z}{\partial \xi}\right)\frac{\partial}{\partial \zeta}\right).$$

In particular, for the two-dimensional case, it is significant that our method is capable of deriving conservative/dissipative, and hence fairly stable, schemes on various domains such as the annular domain; our scheme for the Cahn–Hilliard equation is far more stable than the naive scheme.

Our extension is based on the mapping method. In order to employ this method, we have shown that "the conservation/dissipation properties are obtained from the variational structure" still holds after the change of coordinates. If we could obtain a similar result in space–time, this would make the extension of this type of schemes to the case of moving meshes a possibility; this will be included in future work.

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