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DISCRETE VARIATIONAL DERIVATIVE METHOD—A STRUCTURE-PRESERVING NUMERICAL METHOD FOR PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT. In these decades structure-preserving numerical methods have been developed widely. In general, "structure-preserving" means that the numerical and discrete scheme inherits some mathematical properties from the original differential equation. It means that the design process of a structure-preserving method is a framework to discretize some mathematical properties of equations.

This manuscript describes discrete variational derivative method, which is one of structure-preserving methods for partial/ordinary differential equations. The discrete variational derivative method is a method to design some numerical schemes that inherit some dissipative or conservative properties via discretization of some relationships between the properties and variational structures of ordinary differential equations. We explain some basic concepts of a discrete variational derivative method with some typical examples and show some recent works based on it.

1. Introduction

Discrete variational derivative method, which is a structure-preserving method for partial/ordinal differential equations, is a method to design some numerical schemes that inherit some dissipative or conservative properties from oritinal differential equations via discretization of the variational structure of the equations. In this section, we explain the purpose of the method with an example for the Cahn–Hilliard equation. The Cahn–Hilliard equation is a model equation for a physical and chemical decomposition phenomenon. The phenomenon means that a system with two ingredients transforms itself into two separated phases even its initial state is almost uniform. Spinodal decomposition is used to designate the phenomenon. Typical examples are systems with water and oil, compound polymer systems, and mixed alloy systems. For this phenomenon if we denote the composition ratio distribution function by $u(x,t)$, where x is space variable and t is time, this function $u(x,t)$ becomes a step function essentially where even the initial function $u(x,0)$ is almost constant. This means that the Cahn–Hilliard equation has strong sensitivity to any initial perturbation and strong nonlinearity, and we can understand it is hard to treat for numerical computation.

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For a one dimensional space situation, the Cahn–Hilliard equation is described by

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right),\ x \in (0, L),\ t > 0,\ p < 0,\ q < 0,\ r > 0. \tag{1.1}$$

We note that we restrict our discussion to one dimensional space problems in this manuscript for simplicity. There exist two boundary conditions for the Cahn–Hilliard equation:

$$\frac{\partial u}{\partial x} = \frac{\partial^3 u}{\partial x^3} = 0 \quad \text{at } x = 0, L. \tag{1.2}$$

The first term pu_{xx}, where the coefficient p is negative, in the right-hand side of the Cahn–Hilliard equation means "reverse" diffusion and causes the sensitivity for initial perturbation and numerical instability as we described. We note that $u_{xx} = (\partial/\partial x)^2 u$ and we designate differentiation by subscripts like $u_x = \partial u/\partial x$ hereafter. To have a glance at this instability, let us see some computations by the Euler scheme. For computation, we take the space mesh size is $\Delta x = L/N$ where L is the width of space domain and $N+1$ is the number of the mesh points, and the time mesh size is Δt. The approximate solutions are denoted by ${U_k}^{(m)} \simeq u(k\Delta x, m\Delta t)$ $(k = 0, 1, \ldots, N,\ m = 0, 1, 2, \ldots)$. For convenience, we also denote $\boldsymbol{U}^{(m)} = \left(U_0^{(m)}, \ldots, U_N^{(m)}\right)^\top$ for approximate solutions at time $t = m\Delta t$.

Scheme 1 (The Euler scheme for the Cahn–Hilliard equation)**.** *For a given initial datum $\boldsymbol{U}^{(0)}$, approximate solutions $\boldsymbol{U}^{(m)}$ $(m = 1, 2, \ldots)$ by the Euler scheme should satisfy the following equation:*

$$\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(p\,{U_k}^{(m)} + r\,({U_k}^{(m)})^3 + q\,\delta_k^{\langle 2\rangle}{U_k}^{(m)}\right) \tag{1.3}$$

for $k = 0, \ldots, N$, with two discrete boundary conditions

$$\delta_k^{\langle 1\rangle}{U_k}^{(m)} = \delta_k^{\langle 3\rangle}{U_k}^{(m)} = 0, \quad k = 0, N, \tag{1.4}$$

that correspond to the original conditions (1.2)*. The discrete operators $\delta_k^{\langle p\rangle}$ $(p = 1, 2, 3)$, which are approximations to partial differential operators with second order errors, are defined by $\delta_k^{\langle 1\rangle} f_k = (f_{k+1} - f_{k-1})/(2\Delta x)$, $\delta_k^{\langle 2\rangle} f_k = (f_{k+1} - 2f_k + f_{k-1})/((\Delta x)^2)$, $\delta_k^{\langle 3\rangle} f_k = (f_{k+2} - 2f_{k+1} + 2f_{k-1} - f_{k-2})/(2(\Delta x)^3)$ for a discrete function f_k.*

Some computation results by this Euler scheme are shown in Figure 1. The coefficients of the Cahn–Hilliard equation for the computation are $p = -1.0$, $q = -0.001$, and $r = 1.0$. As the space parameters, $L = 1$, $N = 50$, and $\Delta x = 1/50$. For the time variable, we use two discrete time mesh sizes, $\Delta t = 1/1200$ and $1/12000$. In both graphs, the initial function $u_0(x)$ is indicated by lines, which is close to the x-axis, and defined by

$$u_0(x) = 0.1\sin(2\pi x) + 0.01\cos(4\pi x) + 0.06\sin(4\pi x) + 0.02\cos(10\pi x). \tag{1.5}$$

The numerical solutions with $\Delta t = 1/1200$, which are indicated in the left figure,

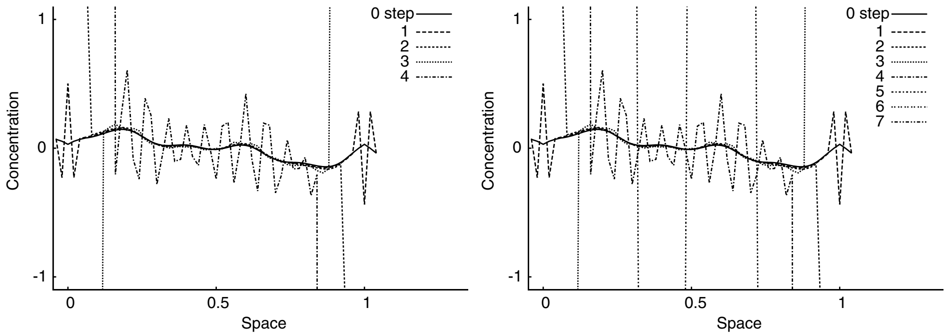

FIGURE 1. Numerical solutions by explicit Euler scheme: left: $\Delta t = 1/1200$; right $\Delta t = 1/12000$.

vibrate and increase rapidly in four or five steps. Even when we take a smaller time mesh size $\Delta t = 1/12000$, the numerical solutions explode in six or seven steps.

We have two counterplans for the instability of numerical solutions. The first plan is to use some stable adaptive methods for ordinary differential equations derived by the method of lines. This plan works well in general, but we have to use quite small time meshes to make computations stable, and the computation cost may be enormous. Another plan is to design some specialized numerical schemes in the target partial differential equation and our aim in this manuscript is to describe a method based on this plan.

To design a specialized scheme for the Cahn–Hilliard equation, we turn our attention to the free (local) energy G:

$$G(u, u_x) \stackrel{\text{def}}{=} \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(u_x)^2. \tag{1.6}$$

The integral of this free energy,

$$J[u] \stackrel{\text{def}}{=} \int_0^L G(u, u_x)\,\mathrm{d}x, \tag{1.7}$$

is called the total energy of the system. Mathematically, the total energy J is a functional of the solution function u. Using the free energy G, the Cahn–Hilliard equation (1.1) and the boundary conditions (1.2) can be described by

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G}{\delta u}\right) \qquad \text{in } x \in [0, L], \tag{1.8}$$

$$\frac{\partial G}{\partial u_x} = \frac{\partial}{\partial x}\left(\frac{\delta G}{\delta u}\right) = 0 \qquad \text{at } x = 0, L, \tag{1.9}$$

where $\delta G/\delta u$ is a variational derivative of $G(u, u_x)$ for u, which satisfies the following relationship with the total energy J:

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

The expression (1.8) using the variational derivative indicates that its solution is a general gradient flow of the system and the system is dissipative. For some discussions later, we describe the dissipation property here.

Proposition 1 (Dissipation property of Cahn–Hilliard equation)**.** *The solution $u(x,t)$ of the Cahn–Hilliard equation satisfies the following inequality:*

$$
\frac{\mathrm{d}}{\mathrm{d}t} J[u] \le 0. \tag{1.11}
$$

Proof. The inequality is proved simply by

$$
\begin{aligned}
(1.12) \qquad \frac{\mathrm{d}}{\mathrm{d}t} J[u] &= \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} \right]_0^L \\
&= -\int_0^L \left(\frac{\partial}{\partial x}\frac{\delta G}{\delta u} \right)^2 \mathrm{d}x + \left[\left(\frac{\delta G}{\delta u} \right) \frac{\partial}{\partial x} \left(\frac{\delta G}{\delta u} \right) \right]_0^L \le 0.
\end{aligned}
$$

We use the discrete boundary condition (1.9) to vanish the boundary term. □

The following important feature of the solution derives this dissipation property.

Proposition 2 (L^∞ boundedness of the Cahn–Hilliard equation)**.** *Let us consider the Cahn–Hilliard equation* (1.1) *with the boundary conditinos* (1.2)*. When the total energy $J[u(\cdot, 0)]$ for the initial state $u(x, 0)$ is finite, the solution $u(x,t)$ of the Cahn–Hilliard equation is bounded:*

$$
\|u(\cdot, t)\|_\infty < \infty, \quad t > 0, \tag{1.13}
$$

where $\|\cdot\|_p$ $(p = 1, 2, \ldots, \infty)$ is a standard L^p norm defined on domain $x \in [0, L]$.

Proof. For any time $t > 0$, we can obtain the following evaluation:

$$
\begin{aligned}
(1.14) \qquad J[u(\cdot, 0)] &\ge J[u(\cdot, t)] = \int_0^L \left\{ \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(u_x)^2 \right\} \mathrm{d}x \\
&\ge \int_0^L \left\{ -pu^2 - \frac{9p^2}{4r} - \frac{1}{2}q(u_x)^2 \right\} \mathrm{d}x \\
&= -p\|u\|_2^2 - \frac{9p^2 L}{4r} - \frac{q}{2}\|u_x\|_2^2
\end{aligned}
$$

by an inequality $(pu^2)/2 + (ru^4)/4 \ge -pu^2 - (9p^2)/(4r)$ and the dissipation property of the total energy (1.12). This means $J[u(\cdot, 0)] + (9p^2 L)/(4r) \ge -p\|u\|_2^2 -$

$(q/2)\|u_x\|_2^2$ and $\|u\|_2, \|u_x\|_2 < \infty$. The boundedness of $\|u\|_2$ and $\|u_x\|_2$ prove this proposition with the Sobolev lemma (e.g., John [33]), which indicates $\|u\|_\infty^2 \leq c\left(\|u\|_2^2 + \|u_x\|_2^2\right)$ for $u(\cdot, t) \in H^1(0, L)$. $\square$

This proposition suggests that **the dissipation property provides the boundedness of the solution** for the Cahn–Hilliard equation. It also suggests that some discrete dissipation properties of numerical schemes may provide some boundedness of numerical solutions. So, we would like to inherit the dissipation property into numerical schemes from the Cahn–Hilliard equation, and this is a typical motivation to design some structure-preserving schemes.

Here, we show a specialized scheme, which inherits the dissipation property of the total energy from the Cahn–Hilliard equation. We, of course, describe how to design such schemes later.

Scheme 2 (A dissipative numerical scheme for the Cahn–Hilliard equation)**.** *For a given initial state $\boldsymbol{U}^{(0)}$, we can obtain numerical solutions $\boldsymbol{U}^{(m)}$ $(m = 1, 2, \ldots)$ by*

$$\begin{aligned}(1.15)\quad &\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t}\\ &\quad = \delta_k^{\langle 2\rangle}\left\{p\left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}\right) + q\delta_k^{\langle 2\rangle}\left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}\right)\right.\\ &\left.+r\left(\frac{({U_k}^{(m+1)})^3 + ({U_k}^{(m+1)})^2{U_k}^{(m)} + {U_k}^{(m+1)}({U_k}^{(m)})^2 + ({U_k}^{(m)})^3}{4}\right)\right\}\end{aligned}$$

for $k = 0, \cdots, N$ with the boundary conditions (1.4)*.*

Let us investigate the dissipation property of this scheme. At first, we define a discrete free energy $G_{\mathrm{d}} : \mathbb{R}^{N+1} \to \mathbb{R}^{N+1}$ by

$$(1.16)\quad G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) \stackrel{\text{def}}{=} \frac{p}{2}({U_k}^{(m)})^2 + \frac{r}{4}({U_k}^{(m)})^2 - \frac{q}{2}\left(\frac{\left(\delta_k^+{U_k}^{(m)}\right)^2 + \left(\delta_k^-{U_k}^{(m)}\right)^2}{2}\right),$$

where $G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})$ means the k-th element of $G_{\mathrm{d}}(\boldsymbol{U}^{(m)})$, δ_k^+ is a forward difference operator defined by $\delta_k^+ f_k = (f_{k+1} - f_k)/\Delta x$, and δ_k^- is a backward one defined by $\delta_k^- f_k = (f_k - f_{k-1})/\Delta x$. We also define the discrete total energy $J_{\mathrm{d}}[\boldsymbol{U}^{(m)}] \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\Delta x$ with the standard trapezoidal summation, which is shown by

$$(1.17)\qquad \sum_{k=0}^{N}{}'' f_k \stackrel{\text{def}}{=} \frac{1}{2}f_0 + f_1 + \cdots + f_{N-1} + \frac{1}{2}f_N.$$

We can find the following discrete dissipation property of this discrete total energy.

Proposition 3 (The discrete dissipation property of total energy for Scheme 2)**.** *The solution of Scheme* 2 *satisfies the following inequality:*

$$J_{\mathrm{d}}[\boldsymbol{U}^{(m+1)}] \leq J_{\mathrm{d}}[\boldsymbol{U}^{(m)}], \quad m = 0, 1, 2, \ldots.$$

We show a generalized dissipation property for Proposition 6 later and its proof is also applicable to this proposition.

Remark 1.1. We use the standard trapezoidal summation rules to approximate integrals in this manuscript, but, of course, we are able to adopt different rules, e.g.. a simple summation rule. We note that the simple summation rule is easier to treat when the boundary condition is periodic.

This discete dissipation property and a discrete Sobolev lemma, which is described later, derive the stability of the numerical solutions.

Proposition 4 (L^∞ boundedness of the numerical solution of Scheme 2)**.** *The solution of Scheme 2 satisfies the following inequality:*

$$\|\boldsymbol{U}^{(m)}\|_\infty \leq 2\left[\frac{\max(1/L, L/2)}{\min(-p,-q/2)}\left\{\sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x + \frac{9p^2 L}{4r}\right\}\right]^{1/2} \tag{1.18}$$

for $m = 0, 1, 2, \cdots$, where $\|\boldsymbol{f}\|_\infty$ is a discrete L^∞ norm that is defined by $\|\boldsymbol{f}\|_\infty \stackrel{\mathrm{def}}{=} \max_{0\leq k\leq N}|f_k|$.

Proof. In similar ways as in the proof for 2, we can show

$$\|\boldsymbol{U}^{(m)}\|_{H^1}^2 \leq \frac{1}{\min(-p,-q/2)}\left\{\sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(0)})\Delta x + \frac{9p^2 L}{4r}\right\} \tag{1.19}$$

where $\|\boldsymbol{f}\|_{H^1} \stackrel{\mathrm{def}}{=} \left(\|\boldsymbol{f}\|^2 + \|\boldsymbol{f}_x\|^2\right)^{1/2}$ is a discete Sobolev norm, $\|\boldsymbol{f}\| \stackrel{\mathrm{def}}{=} \left(\sum_{k=0}^{N}{}''|f_k|^2\Delta x\right)^{1/2}$, and $\|\boldsymbol{f}_x\| \stackrel{\mathrm{def}}{=} \left(\sum_{k=0}^{N-1}|\delta_k^+ f_k|^2\Delta x\right)^{1/2}$. This inequality and the discrete Sobolev lemma, which is described in the next lemma, derive the proposition. □

Lemma 1.2 (Discrete Sobolev lemma)**.** *For any given $\boldsymbol{f} \in \mathbb{C}^{N+1}$, the following inequality is satisfied:*

$$\|\boldsymbol{f}\|_\infty \leq 2\max\left(\frac{1}{\sqrt{L}}, \sqrt{\frac{L}{2}}\right)\|\boldsymbol{f}\|_{H^1}. \tag{1.20}$$

where $L = N\Delta x$,

It is easy to prove this discrete lemma and please refer to Section 8.6 in John [33] or Section 3.6.2 in Furihata and Matsuo [20].

Remark 1.3. As we use the discrete Sobolev lemma to prove Proposition 4, the discrete variational derivative method requires some knowledge about discrete function analysis.

Let us see the numerical solutions by Scheme 2. Figure 2 shows some numerical solutions of the scheme with a rough time mesh $\Delta t = 1/1000$. Other parameters are not different from ones for the explicit Euler scheme. We can find some phase separation phenomena in Figure 2 and it suggests that the numerical solutions behave naturally in the view point of physics or chemistry. We have some experiences for computations with different parameters and initial state, and we have not observed any numerical instability for this scheme. The top figure in Figure 3 shows the discrete total energy with the lapse of time and it indicates the total energy decreases monotonically. For comparison, the total energy by the explicit Euler scheme is shown in the bottom figure and it increases rapidly by its instability.

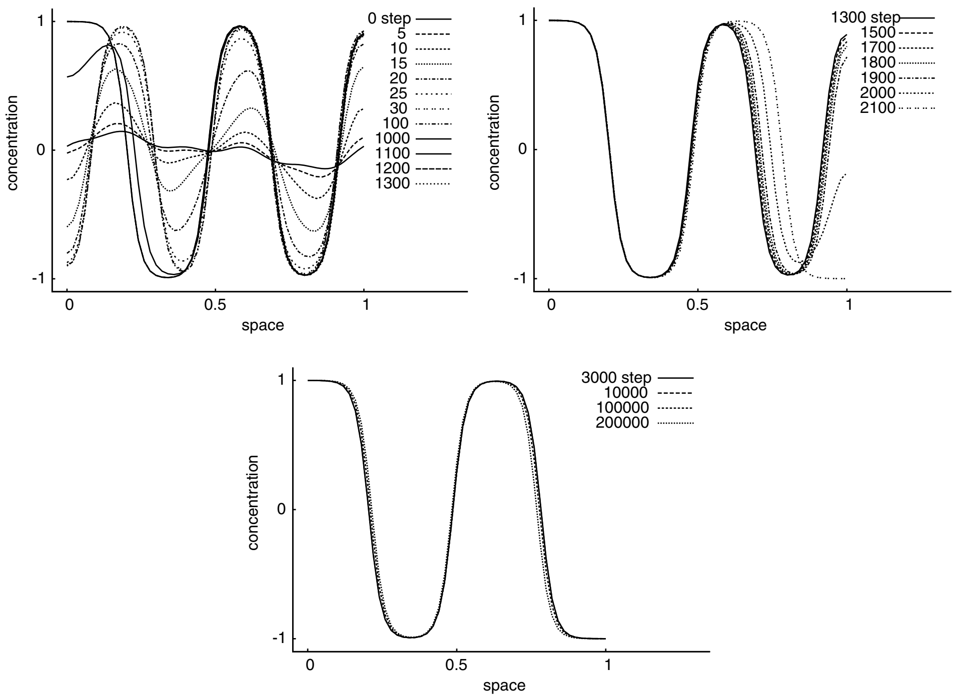

FIGURE 2. The numerical solutions by Scheme 2: left: solutions from 0-th time step to 1300-th; right: from 1300-th to 2100-th; bottom: from 3000-th to 200000-th.

These figures also suggest that the discrete dissipation property of the total energy and the stability of the numerical solution are closely related.

This example for the Cahn–Hilliard equation indicates clearly that some specialized, structure-preserving schemes are superior to other ones. In this case, we guess that the discrete dissipation property contributes the stability of the scheme essentially. For some conservative problems, we also expect that some discrete conservative properties have some "good" side effects to obtain numerical solutions.

2. How to design numerical schemes

In this section, we introduce how to design some structure-preserving schemes in the context of the discrete variational derivative method. We restrict ourselves to a discussion of some typical partial differential equations and omit some cumbersome descriptions for want of space. For detailed definitions and discussions of the discrete variational derivative method, please see Section 3.

2.1. **First order, real-valued differntial equations.** Let us consider some first order, real-valued differential equations. The solution $u(x,t)$ is a real function and we assume that the free energy $G(u,u_x)$ is also a real function. The total energy is defined by $J[u] \stackrel{\text{def}}{=} \int_0^L G(u,u_x)\mathrm{d}x$, which is the same as before. We postpone general discussions to the end of this subsection and treat a typical example partial

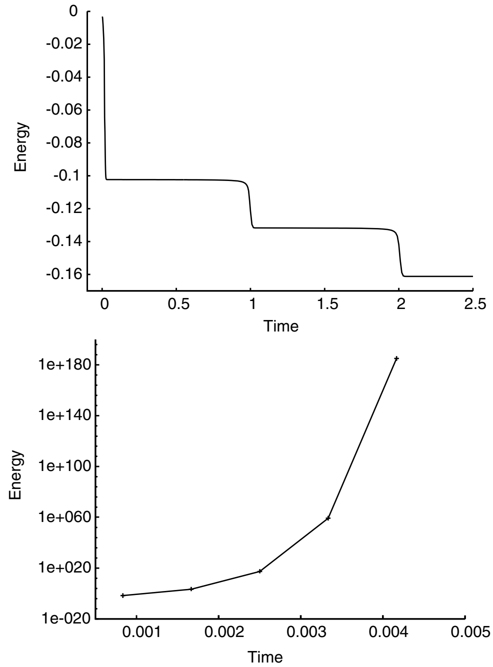

FIGURE 3. The discrete total energy of the numerical solutions: top: total energy by the dissipative Scheme 2; bottom: by the explicit Euler Scheme 1.

differential equation:

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta u}, \quad x \in (0, L),\ t > 0, \tag{2.1}$$

where its boudary conditions satisfy

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_0^L = 0. \tag{2.2}$$

For example, the null-Dirichlet boundary conditions $u(0,t) = u(L,t) = 0$ satisfy this equality. This partial differential equation (2.1) is dissipative in the following sense:

$$\frac{\mathrm{d}}{\mathrm{d}t}J[u] = \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_0^L = -\int_0^L \left(\frac{\delta G}{\delta u}\right)^2 \mathrm{d}x \le 0. \tag{2.3}$$

This dissipation property is indicated by the variational form of the equation (2.1). We note that we may omit some boundary terms in later discussions.

We would like to design some dissipative numerical schemes for this equation. For this purpose, the discrete variational derivative method indicates some procedures to discretize the relationship between the dissipation property and the variational form of the equation (2.1). Applying those procedures, we obtain some dissipative schemes as by-products. These procedures are shown in Figure 4. The left side of the figure indicates the relationship among the free energy, the variational derivative, the partial differential equation, and the dissipation property. We can follow their dependency relations by

step 1: Definition of the free energy G,
step 2: Variational derivative $\delta G/\delta u$ of the free energy for u,
step 3: Definition of the partial differential equation includes the variational derivative,
proposition: Dissipation property of the total energy.

The discrete variational derivative method is essentially to discretize this dependency relation into discrete context. So it is a structure-preserving method literally. The right side of the figure shows the dependency relation in discrete context to be inherited, which can be described by

step 1_{d}: Definition of the *discrete* free energy as an approximation of the original one,
step 2_{d}: *Discrete* variational derivative function,
step 3_{d}: Definition of the *numerical scheme* includes the discrete variational derivative,
proposition: Dissipative property of the *discrete* total energy.

We note that we cannot expect to obtain any numerical scheme that has such dependency relations when we discretize the partial differential equation directly without considering this structure.

Now, let us follow the procedures proposed by the discrete variational derivative method to design some numerical schemes for the partial differential equations (2.1). To see the process in detail, we treat a linear diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{2.4}$$

as a most simple target problem in this case. Taking $G(u, u_x) = (u_x)^2/2$, this diffusion equation is the abstract from equation (2.1). We note that its boundary conditions must satisfy $[u_x u_t]_0^L = 0$.

[step $1_{\mathbf{d}}$] Definition of the *discrete* free energy as an approximation of the original one

We substitute ${U_k}^{(m)}$ for u into $G(u, u_x)$ and some appropriate difference approximations for u_x, and obtain discrete free energy $G_{\mathrm{d}}(\boldsymbol{U}^{(m)})$. The discrete free energy G_{d} is an $(N+1)$ dimensional vector-valued function of $\boldsymbol{U}^{(m)}$ and we denote its element by $G_{\mathrm{d},k}$ for $k = 0, \ldots, N$. We can, of course, use some different difference approximations for u_x, for example, we have

$$(\delta_k^{\langle 1\rangle} {U_k}^{(m)})^2,\ (\delta_k^+ {U_k}^{(m)})^2,\ (\delta_k^- {U_k}^{(m)})^2,\ \frac{(\delta_k^+ {U_k}^{(m)})^2 + (\delta_k^- {U_k}^{(m)})^2}{2}, \tag{2.5}$$

as discrete approximations of ${u_x}^2$. Every discrete approximation can be used in this step, and the acquired scheme should be dissipative. We note that the acquired scheme depends on the approximations in this step, and please see Remark 2.1. Now we adopt a symmetric approximation

$$(u_x)^2 \simeq \frac{(\delta_k^+ {U_k}^{(m)})^2 + (\delta_k^- {U_k}^{(m)})^2}{2} \tag{2.6}$$

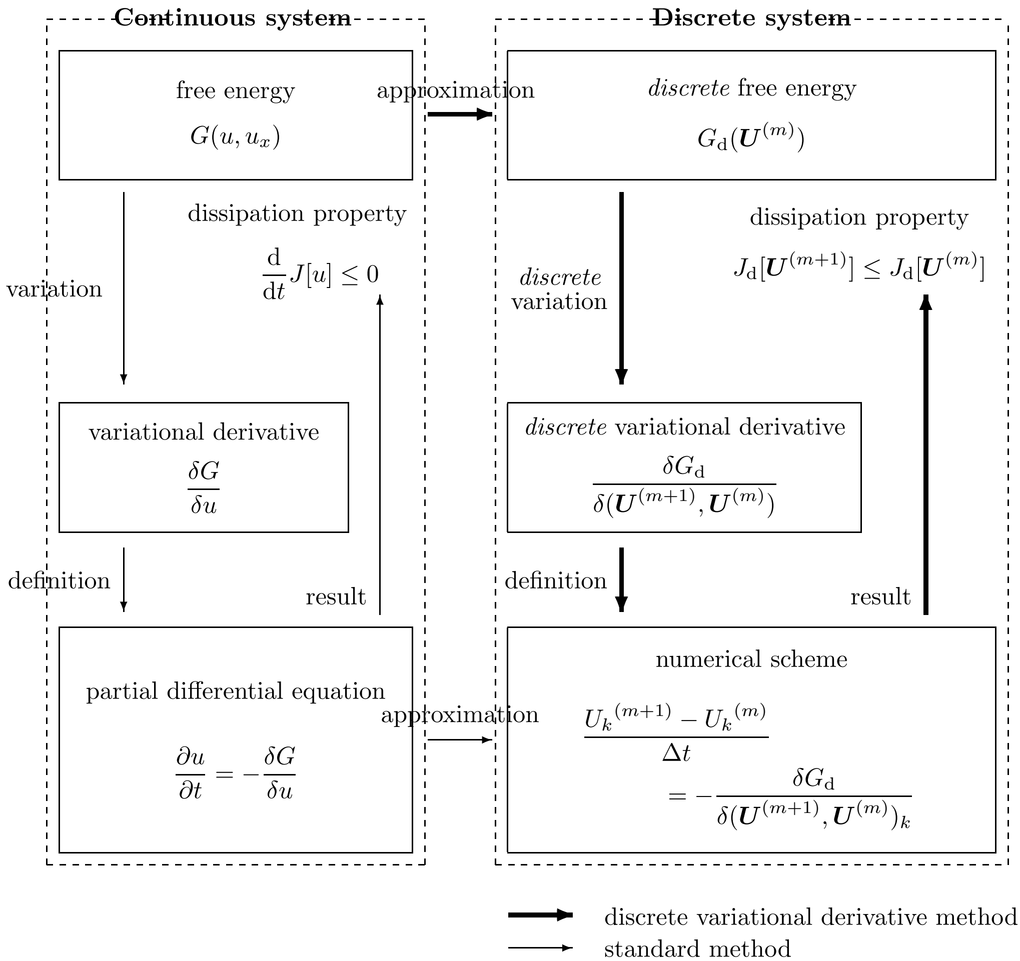

FIGURE 4. Dependency relation to dissipation property and flows to design numerical schemes

for the problem (2.4) and obtain a discrete free energy

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) = \frac{1}{2}\left(\frac{(\delta_k^+ {U_k}^{(m)})^2 + (\delta_k^- {U_k}^{(m)})^2}{2}\right). \tag{2.7}$$

The total energy is defined by $J_{\mathrm{d}}[\boldsymbol{U}^{(m)}] = \sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\Delta x$ using the discrete free energy.

[step $\mathbf{2_d}$] *Discrete* variational derivative function

Here we would like to obtain the discrete variational derivative of the discrete free energy. Some general definitions of the discrete variational derivative are indicated in the next section, and here we derive the derivative through discrete variational calculations to lead the reader to understand. Let us remember that the variation of an integral functional (1.10) is described by

$$\begin{aligned}\int_0^L \{G(u+\delta u, u_x+\delta u_x) - G(u,u_x)\}\,\mathrm{d}x \\ = \int_0^L \frac{\delta G}{\delta u}\delta u\,\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\delta u\right]_0^L + O(\delta u^2).\end{aligned} \tag{2.8}$$

As a similar relation in *discrete context*, discrete variational derivative method requires the following relation:

$$\begin{aligned}&\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x \\ &= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\left({U_k}^{(m+1)} - {U_k}^{(m)}\right)\Delta x + (\text{boundary term})\end{aligned} \tag{2.9}$$

to be satisfied by the discrete variational derivative of G_{d}. For the problem (2.4), we can derive the relation (2.9) easily:

$$\begin{aligned}&\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x \\ &= \frac{1}{2}\sum_{k=0}^{N}{}'' \left(\frac{(\delta_k^+{U_k}^{(m+1)})^2 - (\delta_k^+{U_k}^{(m)})^2}{2} + \frac{(\delta_k^-{U_k}^{(m+1)})^2 - (\delta_k^-{U_k}^{(m)})^2}{2}\right)\Delta x \\ &= \frac{1}{2}\sum_{k=0}^{N}{}'' \left\{\delta_k^+\left(\frac{{U_k}^{(m+1)}+{U_k}^{(m)}}{2}\right)\cdot\delta_k^+({U_k}^{(m+1)} - {U_k}^{(m)})\right. \\ &\qquad \left. +\delta_k^-\left(\frac{{U_k}^{(m+1)}+{U_k}^{(m)}}{2}\right)\cdot\delta_k^-({U_k}^{(m+1)} - {U_k}^{(m)})\right\}\Delta x \\ &= -\sum_{k=0}^{N}{}''\delta_k^{\langle 2\rangle}\left(\frac{{U_k}^{(m+1)}+{U_k}^{(m)}}{2}\right)\cdot({U_k}^{(m+1)} - {U_k}^{(m)})\Delta x + B(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)}),\end{aligned} \tag{2.10}$$

where

$$\begin{aligned}B(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\Bigg[&\delta_k^+\left(\frac{{U_k}^{(m+1)}+{U_k}^{(m)}}{2}\right)\mu_k^+({U_k}^{(m+1)} - {U_k}^{(m)}) \\ &+ \delta_k^-\left(\frac{{U_k}^{(m+1)}+{U_k}^{(m)}}{2}\right)\mu_k^-({U_k}^{(m+1)} - {U_k}^{(m)})\Bigg]_0^N,\end{aligned}$$

$\mu_k^+ f_k \stackrel{\mathrm{def}}{=} (f_{k+1}+f_k)/2$, and $\mu_k^- f_k \stackrel{\mathrm{def}}{=} (f_k+f_{k-1})/2$. In (2.10), we use a symmetric equality $\delta_k^+\delta_k^- = \delta_k^-\delta_k^+ = \delta_k^{\langle 2\rangle}$ and a summation by parts

$$\sum_{k=0}^{N}{}''(\delta_k^+ f_k)g_k\Delta x = -\sum_{k=0}^{N}{}'' f_k(\delta_k^- g_k)\Delta x + \frac{1}{2}\left[(s_k^+ f_k)g_k + f_k(s_k^- g_k)\right]_0^N, \tag{2.11}$$

which corresponds to a discretized integration by parts, where s_k^+, s_k^- are shift operators that are defined by $s_k^+ f_k = f_{k+1}$ and $s_k^- f_k = f_{k-1}$. We describe some general formulas about the summation by parts later. We note that the boundary term $B(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})$ corresponds to the left-hand side of (2.2) and the discrete variational derivative method requires discrete boundary conditions to vanish $B(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})$ for $m = 0, 1, 2, \cdots$ in (2.10).

Now, (2.10) indicates that we can define the discrete variational derivative of G_{d} by

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} = -\delta_k^{\langle 2 \rangle} \left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2} \right) \tag{2.12}$$

naturally, which corresponds to a discretization of the original variational derivative $\delta G/\delta u = -u_{xx}$.

[step $3_{\mathbf{d}}$] Definition of the *numerical scheme* includes the discrete variational derivative

The discrete variational derivative method proposes the following numerical structure-preserving schemes that have abstract formulas using the discrete variational derivative of G_{d}.

Scheme 3 (Dissipative schemes for (2.1))**.** *We assume that given discrete boundary conditions approximate the original boundary conditions and satisfy* $B(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}) = 0$ *for* $m = 0, 1, 2, \cdots$. *For a given initial state* $\boldsymbol{U}^{(0)}$*, the discrete variational derivative method proposes the following scheme:*

$$\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = -\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}, \qquad k = 0, \ldots, N, \tag{2.13}$$

to obtain numerical solution $\boldsymbol{U}^{(m)}$ $(m = 1, 2, \ldots)$ *for the problem* (2.1)*.*

This scheme has a desired dissipation property. The proof for the dissipation property is independent of the concrete form of the free energy G_{d} and the discrete variational derivative of it in a similar manner for the continuous system (2.3).

Proposition 5 (Dissipation property of Scheme 3)**.** *Scheme* 3 *is dissipative in the sense that the total energy decreases, which means:*

$$J_{\mathrm{d}}[\boldsymbol{U}^{(m+1)}] \le J_{\mathrm{d}}[\boldsymbol{U}^{(m)}], \quad m = 0, 1, 2 \ldots. \tag{2.14}$$

Proof. From (2.9), we obtain the following equations:

$$\begin{aligned} (2.15)\quad & J_{\mathrm{d}}[\boldsymbol{U}^{(m+1)}] - J_{\mathrm{d}}[\boldsymbol{U}^{(m)}] \\ = \;& \frac{1}{\Delta t} \sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) \right) \Delta x \\ = \;& \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \left(\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} \right) \Delta x + \frac{B(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})}{\Delta t} \\ = \;& -\sum_{k=0}^{N}{}'' \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \right)^2 \Delta x \le 0. \end{aligned}$$

$\square$

Now, we obtain a concrete expression of a discrete dissipative Scheme 3 for the diffusion equation (2.4) by

$$\frac{U_k{}^{(m+1)} - U_k{}^{(m)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(\frac{U_k{}^{(m+1)} + U_k{}^{(m)}}{2}\right). \tag{2.16}$$

The free energy is (2.7), its discrete variational derivative is (2.12), and the dissipation of total energy is indicated by Proposition 5. As you know, this is a well-known scheme called the Crank–Nicolson scheme. The stability of the Crank–Nicolson scheme is proved by some direct methods like Fourier analysis typically. The discrete variational derivative method also provides a different method to prove the stability. The method uses knowledge of function analysis and the dissipation property. It suggests that the stability analysis of the discrete variational derivative method appears applicable to more complicated, nonlinear problems.

Remark 2.1. As we note in **[step $\mathbf{1_d}$]**, the discrete energy is not unique and a different energy definition may derive a different dissipative scheme. For example, if we define the discrete free energy G_{d} using the approximation $(u_x)^2 \simeq (\delta_k^{\langle 1\rangle} U_k{}^{(m)})^2$ not the former approximation (2.6), then it is defined by

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) = \frac{(\delta_k^{\langle 1\rangle} U_k{}^{(m)})^2}{2} \tag{2.17}$$

and the discrete variational derivative is

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} = -(\delta_k^{\langle 1\rangle})^2\left(\frac{U_k{}^{(m+1)} + U_k{}^{(m)}}{2}\right). \tag{2.18}$$

So, the obtained numerical scheme is

$$\frac{U_k{}^{(m+1)} - U_k{}^{(m)}}{\Delta t} = (\delta_k^{\langle 1\rangle})^2\left(\frac{U_k{}^{(m+1)} + U_k{}^{(m)}}{2}\right). \tag{2.19}$$

This scheme is different from the former scheme (2.16), but also “dissipative” in the sense that the total energy for the free energy $G_{\mathrm{d}}(\boldsymbol{U}^{(m)})$ (2.17) satisfies Proposition 5.

As this example indicates, we can define the discrete free energy arbitrarily in the discrete variational derivative method. Once we define the discrete free energy, the discrete dissipative/conservative numerical method will be derived almost automatically. Some important features of the obtained schemes, e.g., stability, depend on their concrete forms much, and it means that we should select the definition of the discrete free energy carefully.

Here we generalize the discrete variational derivative method for some first order differential equations from the discussion about the diffusion equation.

First order, real-valued dissipative equations. Let us consider the following general partial differential equations:

$$\frac{\partial u}{\partial t} = (-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s}\frac{\delta G}{\delta u}, \qquad s = 0, 1, 2, \cdots, \tag{2.20}$$

which has some boundary conditions that satisfy

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \sum_{l=1}^{s}(-1)^{s+l}F^{\langle l-1\rangle}F^{\langle 2s-l\rangle}\right]_0^L = 0 \tag{2.21}$$

for $t > 0$, where the second term is zero when $s = 0$ and $F^{\langle l \rangle} \stackrel{\mathrm{def}}{=} (\partial/\partial x)^l (\delta G/\delta u)$. These equations are dissipative, i.e., the total energy $J[u] = \int_0^L G(u, u_x)\mathrm{d}x$ decreases. The diffusion equation and the Allen–Cahn equation [1] are the partial differential equations (2.20) with $s = 0$, and the Cahn–Hilliard equation and the prominence temperature equation [2, pp.7–8] are ones with $s = 1$.

The discrete variational derivative method proposes a numerical scheme:

$$\frac{U_k{}^{(m+1)} - U_k{}^{(m)}}{\Delta t} = (-1)^{s+1} \delta_k^{\langle 2s \rangle} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \right) \tag{2.22}$$

for the problem (2.21), where $\delta_k^{\langle h \rangle}$ is an h-th order central difference operator, which is defined in Proposition 7 to be described. The discrete variational derivative method requires the boundary conditions to satisfy

$$\frac{B_{\mathrm{r},1}(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})}{\Delta t} + (-1)^{s+1} B_{\mathrm{r},2}^{\langle 2s \rangle}(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}) = 0. \tag{2.23}$$

We note that this requirement corresponds to (2.21). $B_{\mathrm{r},1}(\cdot,\cdot)$ is defined in (3.8) and $B_{\mathrm{r},2}^{\langle 2s \rangle}(\cdot,\cdot)$ is defined by

$$\begin{aligned} &B_{\mathrm{r},2}^{\langle 2s \rangle}(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}) \stackrel{\mathrm{def}}{=} \\ &\Bigg[-\sum_{\substack{1 \le l \le s \\ l:\mathrm{even}}} \frac{2\varphi_k^{\langle l-1 \rangle} \varphi_k^{\langle 2s-l \rangle} + \left(\delta_k^+ \varphi_k^{\langle l-2 \rangle}\right)\left(s_k^+ \varphi_k^{\langle 2s-l \rangle}\right) + \left(\delta_k^- \varphi_k^{\langle l-2 \rangle}\right)\left(s_k^- \varphi_k^{\langle 2s-l \rangle}\right)}{4} \\ &+ \sum_{\substack{1 \le l \le s \\ l:\mathrm{odd}}} \frac{2\varphi_k^{\langle l-1 \rangle} \varphi_k^{\langle 2s-l \rangle} + \left(s_k^+ \varphi_k^{\langle l-1 \rangle}\right)\left(\delta_k^+ \varphi_k^{\langle 2s-l-1 \rangle}\right) + \left(s_k^- \varphi_k^{\langle l-1 \rangle}\right)\left(\delta_k^- \varphi_k^{\langle 2s-l-1 \rangle}\right)}{4} \Bigg]_0^N \end{aligned} \tag{2.24}$$

where $\varphi_k^{\langle l \rangle} \stackrel{\mathrm{def}}{=} \delta_k^{\langle l \rangle} \left(\delta G_{\mathrm{d}} / \delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k \right)$. The proposed numerical scheme (2.22) is dissipative.

Proposition 6 (Dissipation property of the general scheme (2.22))**.** *Assuming that discrete boundary conditions satisfy* (2.23)*, the scheme* (2.22) *is dissipative in the sense that the discrete total energy decreases:*

$$J_{\mathrm{d}}[\boldsymbol{U}^{(m+1)}] \le J_{\mathrm{d}}[\boldsymbol{U}^{(m)}], \quad m = 0, 1, 2, \cdots.$$

Proof. We obtain the following inequality using a discrete variational equality (3.7) and Proposition 9 about higher summation by parts in the next section:

$$
\begin{aligned}
(2.25)\qquad & \frac{1}{\Delta t}\sum_{k=0}^{N}{}''\{G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\}\Delta x \\
= \ & \sum_{k=0}^{N}{}''\left[\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right)\left(\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t}\right)\right]\Delta x \\
& \qquad + \frac{B_{\mathrm{r},1}(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})}{\Delta t} \\
= \ & \sum_{k=0}^{N}{}''\left[\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right)\cdot(-1)^{s+1}\delta_k^{\langle 2s\rangle}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right]\Delta x \\
& \qquad + \frac{B_{\mathrm{r},1}(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})}{\Delta t} \\
= \ & -\sum_{k=0}^{N}{}''\Psi_k^{(s)}\Delta x + \frac{B_{\mathrm{r},1}(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})}{\Delta t} + (-1)^{s+1}B_{\mathrm{r},2}^{\langle 2s\rangle}(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)}) \le 0,
\end{aligned}
$$

where $\Psi_k^{(s)} \stackrel{\mathrm{def}}{=} (\varphi_k^{\langle s\rangle})^2$ (when s is even), and $\left\{(\delta_k^+\varphi_k^{\langle s-1\rangle})^2 + (\delta_k^-\varphi_k^{\langle s-1\rangle})^2\right\}/2$ (when s is odd). The proposition is satisfied since the discrete boundary conditions vanish the boundary terms and $\Psi_k^{(s)}$ is nonnegative. □

Actually, the dissipative Scheme 2 for the Cahn–Hilliard equation is the generalized scheme (2.22) with the discrete free energy G_{d} in (1.16), and its stability is proved by Proposition 6. To confirm this comment, the definition of the discrete variational derivative (3.6) may help the reader.

First order, real-valued conservative equations. The following partial differential equations:

$$
(2.26)\qquad \frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{2s+1}\frac{\delta G}{\delta u}, \qquad s = 0,1,2\cdots,
$$

are conservative in the sense that the system conserves the total energy $J[u] = \int_0^L G(u,u_x)\mathrm{d}x$ under appropriate boundary conditions. The discussion about the boundary conditions is about the same as that for dissipative equations, and we omit it.

The well-known Korteweg–de Vries equation [36] and the Zakharov–Kuznetsov equation [60] are examples of this problem. The discrete variational derivative method proposes the following numerical scheme for this generalized conservative equations:

$$
(2.27)\qquad \frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = \delta_k^{\langle 2s+1\rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right).
$$

We have indicated that this scheme conserves the discrete total energy $J_{\mathrm{d}}[\boldsymbol{U}^{(m)}] = \sum_{k=0}^{N}{}''G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\Delta x$ under appropriate discrete boundary conditions.

Remark 2.2. We can expand these discussions considering a more generalized differential equation:

$$\frac{\partial u}{\partial t} = \mathcal{A}\,\frac{\delta G}{\delta u}, \tag{2.28}$$

where $\mathcal{A}$ is an operator. When the operator $\mathcal{A}$ is negative-definite for the natural inner product derived by integration, the system is dissipative. If the operator is skew-symmetric, then the system is conservative. So, the discrete variational derivative method is expanded to design some numerical schemes that inherit the negative-definite property or the skew-symmetric property of the operator $\mathcal{A}$.

Remark 2.3. Expanding the formulation of the free energy, e.g., domain of definition, provides more target differential equations for the discrete variational derivative method. For example, if we consider the free energy function written by $G = G(u, u_x, u_{xx})$, then we can treat the Swift–Hohenberg equation [53] as a first order, real-valued dissipative equation (2.20). When we consider $G = G(u, \mathcal{H}^{-1}u)$, where $\mathcal{H}$ is the Helmholtz operator, we can apply the discrete variational derivative method to the Keller–Segel equation [34] as a dissipative problem.

2.2. **First order, complex-valued differential equations.** For some complex-valued differential equations, we are able to discuss the discrete variational derivative method in a similar manner. Assuming that the solution $u(x,t)$ is a complex-valued function and the free energy $G(u, u_x)$ is a real-valued function, we can define the variational derivative functions by

$$\frac{\delta G}{\delta u} \stackrel{\text{def}}{=} \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}, \qquad \frac{\delta G}{\delta \overline{u}} \stackrel{\text{def}}{=} \frac{\partial G}{\partial \overline{u}} - \frac{\partial}{\partial x}\frac{\partial G}{\partial \overline{u_x}},$$

where $\overline{u}$ is the complex conjugate of u and obtain the following variational equality:

$$\begin{aligned} &\int_0^L (G(u+\delta u, u_x + \delta u_x) - G(u, u_x))\mathrm{d}x \\ &= \int_0^L \left(\frac{\delta G}{\delta u}\delta u + \frac{\delta G}{\delta \overline{u}}\delta\overline{u}\right)\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\delta u + \frac{\partial G}{\partial \overline{u_x}}\delta \overline{u}\right]_0^L + O(|\delta u|^2). \end{aligned} \tag{2.29}$$

Using these equalities, we can design some structure-preserving schemes for some problems, for example, the following differential equation.

First order, complex-valued dissipative equation. Let us consider the following partial differential equation:

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \tag{2.30}$$

where its boundary conditions satisfy

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

for $t > 0$. It is not difficult to confirm that this equation is dissipative, i.e., the total energy $J[u] = \int_0^L G(u, u_x)\mathrm{d}x$ descreases, by

$$\frac{\mathrm{d}}{\mathrm{d}t}J[u] = -2\int_0^L \left|\frac{\delta G}{\delta u}\right|^2 \mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u}}{\partial t}\right]_0^L \leq 0.$$

A variant of the Ginzburg–Landau equation [38], which is a model equation for the super-conductivity phenomenon, and the Newell–Whitehead equation [47], which is a model for the Bénard flow, are examples that we can treat as the complex-valued dissipative equation and compute some numerical solutions by the discrete variational derivative method [20]. We omit any detailed discussion of them.

First order, complex-valued conservative equation. The following partial differential equation:

$$i\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}} \tag{2.31}$$

is conservative with some appropriate boundary conditions. The requirement for the boundary conditions is the same as that in the former case. The conservation property is indicated by

$$\frac{\mathrm{d}}{\mathrm{d}t}J[u] = \int_0^L \left(i\left|\frac{\delta G}{\delta u}\right|^2 - i\left|\frac{\delta G}{\delta u}\right|^2 \right) \mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u}}{\partial t} \right]_0^L = 0.$$

We can apply this context to the well-known nonlinear Schrödinger equation [5, 51] and the Gross–Pitaevskii equation [26, 48], which is a model of the Bose–Einstein condensation, and obtain their numerical solutions by the discrete variational derivative method.

2.3. **Other partial differential equations.** There exist lots of partial differential equations that are different from the equations described so far, and we can apply the discrete variational derivative method. For example, some systems of differential equations are dissipative or conservative, and the discrete variational derivative method derives some structure-preserving schemes for them. We omit the general discussion, which is described in Section 2.4 in Furihata and Matsuo [20], and give examples. The "good" Boussinesq equation [40]:

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix}\begin{pmatrix} \delta G/\delta u \\ \delta G/\delta v \end{pmatrix}, \tag{2.32}$$

where $G(u, u_x, v, v_x) = u^2/2 + u^3/3 + (u_x)^2/2 + v^2/2$, is a typical conservative system of equations that we can design using the discrete variational derivative method scheme. As other examples of the conservative systems, we can cite the Zakharov equation [21, 59], standard Hamilton systems, the Boussinesq–Schrödinger equation [4], the coupled Klein–Gordon–Schrödinger equation [3], and the long-short wave interaction equation [58]. The Eguchi–Oki–Matsumura equation [13] and a variant of the Ginzburg–Landau equation [11] are examples of the dissipative systems that we can apply the discrete variational derivative method.

Second order partial differential equations. The following second order partial differential equation:

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta G}{\delta u} \tag{2.33}$$

is also conservative and one of the target equations for the discrete variational derivative method. We require that the boundary conditions satisfy $[(\partial G/\partial u_x)\,(\partial u/\partial t)]_0^L = 0$. We should note that the definition of the total energy of this problem is

$$J[u] \stackrel{\text{def}}{=} \int_0^L \left\{ (u_t)^2/2 + G(u, u_x) \right\} \mathrm{d}x, \tag{2.34}$$

and different from that for other problems. The conservation property is indicated by

$$\frac{\mathrm{d}}{\mathrm{d}t}J[u] = \int_0^L \left(u_{tt} + \frac{\delta G}{\delta u} \right) u_t \,\mathrm{d}x + \left[\frac{\partial G}{\partial u_x} \frac{\partial u}{\partial t} \right]_0^L = 0.$$

This second order abstract equation also includes lots of concrete target problems, for example, the Fermi–Pasta–Ulam equation [15], the nonlinear string vibration equation [9], the nonlinear Klein–Gordon equation [16, 17, 24, 35], the Shimoji–Kawai equation [50], and the Ebihara equation [12]. The discrete variational derivative method proposes two approaches for this equation. The first approach is to introduce a new dependent variable, decrease the differentiation order to first order, and treat a system of first order differential equations equivalent to the original second order equation. Another one is to define the discrete free energy G_{d} by $G_{\mathrm{d}} = G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})$, and define the discrete total energy by

$$J_{\mathrm{d}}[\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}] \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' \left\{ \frac{1}{2} \left(\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} \right)^2 + G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}) \right\} \Delta x,$$

and apply the discrete variational derivative method using these definitions.

3. Detailed definitions and discussion

In this section, we describe the summation by parts, discrete variational derivative and some detailed notation, which is required to understand the process of the discrete variational derivative method in detail. By the mathematical definition of the discrete variational derivative, we can avoid some vagueness of computation of them. We restrict our discussion to real-valued equations to avoid cumbersome descriptions in this section. We describe more detailed discussions and treatments of complex-valued equations in Furihata and Matsuo [20]and ask the reader to refer it.

3.1. Summation by parts.

For general discussion using some difference operators, there exists a significant mathematical obstacle. The definitions of even order difference operators are different from that of odd order operators. To dissolve this obstacle, we indicate the following proposition.

Proposition 7 (General expression of the central difference operators)**.** *We can denote the h-th order central difference operators $\delta_k^{\langle h \rangle}$ by an expression:*

$$\delta_k^{\langle h \rangle} = \boldsymbol{e}^{\mathrm{T}} D_k^h \,\boldsymbol{e}, \qquad h = 0, 1, 2, \cdots, \tag{3.1}$$

where

$$D_k \stackrel{\text{def}}{=} \begin{pmatrix} 0 & \delta_k^+ \\ \delta_k^- & 0 \end{pmatrix}, \qquad \boldsymbol{e} \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

and $D_k^0 \stackrel{\text{def}}{=} I$.

Proof. Using that $\delta_k^{\langle h \rangle} = (\delta_k^{\langle 2 \rangle})^{h/2}$ for even h and $\delta_k^{\langle h \rangle} = (\delta_k^{\langle 2 \rangle})^{(h-1)/2}\,\delta_k^{\langle 1 \rangle}$ for odd h, the proposition is proved immediately. ☐

Based on this proposition, we can derive some concrete expressions of summation by parts from the following general summation by parts.

Proposition 8 (General expression of summation by parts). *In general, the following equality is satisfied:*

$$\sum_{k=0}^{N}{}'' \left\{ a_k D_k a'_k + (D_k a_k^{\mathsf{T}})^{\mathsf{T}} a'_k \right\} \Delta x = \frac{1}{2} \left[a_k A_k a'_k + (A_k a_k^{\mathsf{T}})^{\mathsf{T}} a'_k \right]_{k=0}^{N}, \tag{3.2}$$

where

$$a_k \stackrel{\text{def}}{=} \begin{pmatrix} \zeta_k & \eta_k \\ \theta_k & \xi_k \end{pmatrix}, \qquad a'_k \stackrel{\text{def}}{=} \begin{pmatrix} \zeta'_k & \eta'_k \\ \theta'_k & \xi'_k \end{pmatrix}, \qquad A_k \stackrel{\text{def}}{=} \begin{pmatrix} 0 & s_k^+ \\ s_k^- & 0 \end{pmatrix},$$

and $\{\zeta_k\}$, $\{\eta_k\}$, $\{\theta_k\}$, $\{\xi_k\}$, $\{\zeta'_k\}$, $\{\eta'_k\}$, $\{\theta'_k\}$, $\{\xi'_k\}$ *are arbitrary scalar sequences.*

Proof. We can confirm this equality of each element using the most simple summation by parts (2.11). $\square$

This general expression derives the following high order summation by parts, which is required for the general discrete variational derivative method.

Proposition 9 (High order summation by parts). *Assume* $s \in \{1, 2, 3, \cdots\}$. *For even* s, *the following summaton by parts is satisfied:*

$$\begin{aligned}
\sum_{k=0}^{N}{}'' f_k \delta_k^{\langle s \rangle} f_k \Delta x &= (-1)^{s/2} \sum_{k=0}^{N}{}'' F_k^{(s,s/2)} \Delta x \\
&+ \Bigg[- \sum_{\substack{1 \le l \le s/2 \\ l:\text{even}}} \frac{2 f_k^{\langle l-1 \rangle} f_k^{\langle s-l \rangle} + \left(\delta_k^+ f_k^{\langle l-2 \rangle} \right) \left(s_k^+ f_k^{\langle s-l \rangle} \right) + \left(\delta_k^- f_k^{\langle l-2 \rangle} \right) \left(s_k^- f_k^{\langle s-l \rangle} \right)}{4} \\
&\quad + \sum_{\substack{1 \le l \le s/2 \\ l:\text{odd}}} \frac{2 f_k^{\langle l-1 \rangle} f_k^{\langle s-l \rangle} + \left(s_k^+ f_k^{\langle l-1 \rangle} \right) \left(\delta_k^+ f_k^{\langle s-l-1 \rangle} \right) + \left(s_k^- f_k^{\langle l-1 \rangle} \right) \left(\delta_k^- f_k^{\langle s-l-1 \rangle} \right)}{4} \Bigg]_0^N,
\end{aligned}$$

where $f_k^{\langle l \rangle} \stackrel{\text{def}}{=} \delta_k^{\langle l \rangle} f_k$, *and*

$$F_k^{(l,l')} \stackrel{\text{def}}{=} \begin{cases} f_k^{\langle l' \rangle} s_k^{\langle l \bmod 2 \rangle} f_k^{\langle l' \rangle} & : \textit{when } l' \textit{ is even}, \\ \dfrac{1}{2} \left\{ \left(\delta_k^+ f_k^{\langle l'-1 \rangle} \right)^2 + \left(\delta_k^- f_k^{\langle l'-1 \rangle} \right)^2 \right\} & : \textit{when } l' \textit{ is odd}, \end{cases} \tag{3.3}$$

for $l, l' \in \{0, 1, 2, \ldots\}$. *For odd* s, *the follwing equation is satisfied:*

$$\begin{aligned}
\sum_{k=0}^{N}{}'' f_k \delta_k^{\langle s \rangle} f_k \Delta x &= \\
&\Bigg[- \sum_{\substack{1 \le l \le (s-1)/2 \\ l:\text{even}}} \frac{\left(\delta_k^+ f_k^{\langle l-2 \rangle} \right) \left(\delta_k^+ f_k^{\langle s-l-1 \rangle} \right) + \left(\delta_k^- f_k^{\langle l-2 \rangle} \right) \left(\delta_k^- f_k^{\langle s-l-1 \rangle} \right)}{2} \\
&+ \sum_{\substack{1 \le l \le (s-1)/2 \\ l:\text{odd}}} \frac{f_k^{\langle l-1 \rangle} \left(s_k^{\langle 1 \rangle} f_k^{\langle s-l \rangle} \right) + \left(s_k^{\langle 1 \rangle} f_k^{\langle l-1 \rangle} \right) f_k^{\langle s-l \rangle}}{2} + \frac{1}{2} (-1)^{(s-1)/2} F_k^{(s,(s-1)/2)} \Bigg]_0^N.
\end{aligned}$$

Proof. Proposition 8 indicates

$$\sum_{k=0}^{N}{}'' \left\{ a_k D_k^h a'_k \right\} \Delta x = (-1)^{h'} \sum_{k=0}^{N}{}'' \left(D_k^{h'} a_k^{\mathsf{T}} \right)^{\mathsf{T}} \left(D_k^{h-h'} a'_k \right) \Delta x$$
$$+\frac{1}{2} \left[\sum_{l=1}^{h'} (-1)^{l-1} \left\{ \left(D_k^{l-1} a_k^{\mathsf{T}}\right)^{\mathsf{T}} \left(A_k D_k^{h-l} a'_k\right) + \left(A_k D_k^{l-1} a_k^{\mathsf{T}}\right)^{\mathsf{T}} \left(D_k^{h-l} a'_k\right) \right\} \right]_{k=0}^{N}$$

for $0 \le h' \le h$. Operating the $\boldsymbol{e}$ to both sides of this expression, we obtain a scalar equation that corresponds to the proposition. □

3.2. **Discrete variational derivative.** Here, we indicate the mathematical definition of the discrete variational derivative. For simplicity, we assume that the free energy is a real-valued function $G = G(u, u_x)$ that depends only on a real-valued function u and the derivative u_x and we can describe it by

$$G(u, u_x) = \sum_{l=1}^{\widetilde{M}} \widetilde{f}_l(u) \widetilde{g}_l(u_x), \quad \widetilde{M} \in \mathbb{N}, \tag{3.4}$$

where $\{\widetilde{f}_l, \widetilde{g}_l\}_{l=1}^{\widetilde{M}}$ are real-valued differentiable functions. We also assume that we define the discrete energy function by

$$G_{\mathrm{d},k}(\boldsymbol{U}) = \sum_{l=1}^{M} f_l(U_k) g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k), \quad k = 0, \cdots, N, \tag{3.5}$$

where $\{f_l, g_l^{\pm}\}_{l=1}^{M}$ are differentiable functions. The discrete free energy G_{d}, of course, should approximate the original free energy G. Under these assumptions, the discrete variational derivative method provides the definition of the discrete variational derivative of G_{d}.

Definition of discrete variational derivative. The definition of the discrete variational derivative of the discrete free energy G_{d} (3.5) for $\boldsymbol{U}, \boldsymbol{V} \in \mathbb{R}^{N+1}$ is

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})_k} \stackrel{\mathrm{def}}{=} \frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U}, \boldsymbol{V})_k} - \delta_k^- \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^+(\boldsymbol{U}, \boldsymbol{V})_k} \right) - \delta_k^+ \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^-(\boldsymbol{U}, \boldsymbol{V})_k} \right) \tag{3.6}$$

for $k = 0, \cdots, N$, where

$$\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U}, \boldsymbol{V})_k} \stackrel{\mathrm{def}}{=} \sum_{l=1}^{M} \left(\frac{f_l(U_k) - f_l(V_k)}{U_k - V_k} \right) \left(\frac{g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k) + g_l^+(\delta_k^+ V_k) g_l^-(\delta_k^- V_k)}{2} \right),$$

$$\frac{\partial G_{\mathrm{d}}}{\partial \delta^-(\boldsymbol{U}, \boldsymbol{V})_k}$$
$$\stackrel{\mathrm{def}}{=} \sum_{l=1}^{M} \left(\frac{f_l(U_k) + f_l(V_k)}{2} \right) \left(\frac{g_l^+(\delta_k^+ U_k) + g_l^+(\delta_k^+ V_k)}{2} \right) \left(\frac{g_l^-(\delta_k^- U_k) - g_l^-(\delta_k^- V_k)}{\delta_k^-(U_k - V_k)} \right),$$

$$\frac{\partial G_{\mathrm{d}}}{\partial \delta^+(\boldsymbol{U}, \boldsymbol{V})_k}$$
$$\stackrel{\mathrm{def}}{=} \sum_{l=1}^{M} \left(\frac{f_l(U_k) + f_l(V_k)}{2} \right) \left(\frac{g_l^-(\delta_k^- U_k) + g_l^-(\delta_k^- V_k)}{2} \right) \left(\frac{g_l^+(\delta_k^+ U_k) - g_l^+(\delta_k^+ V_k)}{\delta_k^+(U_k - V_k)} \right).$$

This definition should satisfy the relation (2.9).

Proposition 10 (Discrete variation)**.** *For any $\boldsymbol{U}, \boldsymbol{V} \in \mathbb{R}^{N+1}$, the discrete free energy* (3.5) *and the discrete variational derivative* (3.6) *satisfy the following equality:*

$$\begin{aligned} &\sum_{k=0}^{N}{}'' \left\{ G_{\mathrm{d},k}(\boldsymbol{U}) - G_{\mathrm{d},k}(\boldsymbol{V}) \right\} \Delta x \\ &\quad = \sum_{k=0}^{N}{}'' \left[\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} \right) (U_k - V_k) \right] \Delta x + B_{\mathrm{r},1}(\boldsymbol{U},\boldsymbol{V}), \end{aligned} \tag{3.7}$$

where

$$\begin{aligned} &B_{\mathrm{r},1}(\boldsymbol{U},\boldsymbol{V}) \\ &\stackrel{\mathrm{def}}{=} \frac{1}{2} \left[\frac{\partial G_{\mathrm{d}}}{\partial \delta^{+}(\boldsymbol{U},\boldsymbol{V})_k} (s_k^{+}(U_k - V_k)) + \left\{ s_k^{-} \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^{+}(\boldsymbol{U},\boldsymbol{V})_k} \right) \right\} (U_k - V_k) \right. \\ &\qquad \left. + \frac{\partial G_{\mathrm{d}}}{\partial \delta^{-}(\boldsymbol{U},\boldsymbol{V})_k} (s_k^{-}(U_k - V_k)) + \left\{ s_k^{+} \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^{-}(\boldsymbol{U},\boldsymbol{V})_k} \right) \right\} (U_k - V_k) \right]_0^N . \end{aligned} \tag{3.8}$$

4. Advanced topics and summary

For the reader, we mention some advanced topics of the discrete variational derivative method and describe a summary.

4.1. **Advanced topics.**

From Furihata and Matsuo [20], we extract some advanced topics of the discrete variational derivative method.

Schemes with high accuracy. In general, a numerical scheme using the standard central difference operators is second order in the sense of accuracy. There exist some approaches to design some numerical schemes with higher accuracy. One is to use higher accurate operators simply. This idea works well for the accuracy for the space discretization, but it is hard to design numerical schemes to be accurate for the time discretization. Moreover, the obtained scheme with high accuracy for the time discretization may cost significantly. Another approach is the composition method [52, 57]. This approach works well, and its implementation is not difficult, but the composition method requires some "reverse-time computation process" and every discrete dissipation property is ruined theoretically by this process.

Schemes with low computation cost. Applying the standard discrete variational derivative method to nonlinear partial differential equations, we obtain nonlinear schemes in general. The order of nonlinearity of the scheme is the same as of the original equation, e.g., the numerical scheme should be a cubic polynomial of $\boldsymbol{U}^{(m+1)}$ for a differential equation that is a cubic polynomial of $u(x,t)$. This means that the computation cost to obtain $\boldsymbol{U}^{(m+1)}$ may be significant for highly nonlinear problems. We have developed a method to decrease the order of nonlinearity of the scheme introducing extra time steps. The introduction of extra time steps may unstabilize the schemes in general, so this method demands lots of care to apply.

Galerkin approach. We describe the finite difference schemes of the discrete variational derivative method in this manuscript. We can, of course, apply the approach to problems based on the methods used in the finite element Galerkin method. The Galerkin approach is quite flexible about the space discretization and easy to handle for the problems with high space dimensions. However, taking some function spaces that conforms to each other may be difficult when the order of differentiation is high.

Mesh configuration. The discrete variational derivative method requires some discrete mathematical relations, e.g., the summation by parts and the discrete Green's theorem, between differential operations and integration. However, those relations depend on the mesh shapes in general. This dependency has been a fatal obstacle to the discrete variational derivative method on some flexible mesh shapes. Recently, some approaches, e.g., the Galerkin approach and generalized discrete Green's theorem, relaxes this difficulty.

4.2. **Summary.** We describe the basic ideas, features, and definitions of the discrete variational derivative method which is a structure-preserving method for some dissipative or conservative partial differential equations. The essence of the method is the discretization of the dependency relation among the free energy, the variational derivative, the partial differential equation, and the dissipation property. The idea is simple to understand and also applicable to lots of concrete problems. Some notation in the finite difference context may be cumbersome, but it may not bother the reader since the concrete expressions are easier to treat. We, the authors, hope that this manuscript will help the reader with the numerical computations or the structure-preserving methods.

Appendix: History. Here we will briefly introduce the studies related to the structure-preserving methods. The early attempts to inherit some features from the equations are studies about ordinary differential equations. For example, in the 1970s Greenspan [25] show a discrete conservative scheme for a conservative dynamical system. Gonzalez [22] and McLachlan–Quispel–Robidoux [45] later expanded it to the general dynamical systems. The symplectic method for the Hamilton system is a quite well known structure-preserving method for ordinary differential equations and considerably superior to the numerical methods. Hairer–Lubich–Wanner [28], Sanz-Serna and Calvo [49], and Leimkuhler–Reich [37] will help the reader to understand the symplectic method. The works in Faou–Hairer–Pham [14] and Hairer [27] show some other relaxed conservative methods. We can read the excellent and comprehensive reviews on the development of the numerical methods, sometimes called "geometric integration for ordinary differential equations", in Hairer–Lubich–Wanner [28] and Budd–Piggott [7].

For partial differential equations, we can find some early studies from the 1970s. We refer the reader to section 1.2 in Furihata and Matsuo [20] for some general approaches, which include the discrete variational derivative method developed in the 1990s. Furihata–Mori [18, 19] proposed the discrete variational derivative method in 1996 and 1999, and many authors [31, 43, 44, 55, 56] have developed the method. Furihata and Matsuo [20] is a reference to describe the development. Around the same time, Gonzalez [23] proposed a conservative method for some general problems describing deformation elastodynamics, which is based on a special technique in time discretization [22]. Other excellent works to design conservative schemes, e.g., in Mclachlan–Robidoux [46], are also based on their studies on ordinary differential equations [45]. Jiménez [32] also studies a systematic approach to designing some discrete conservation schemes. Concerning the relaxed conservation or dissipation properties, there exist some interesting approaches and Budd–Piggot [7] is an appropriate review. For Hamiltonian partial differential equations, Marsden–Patrick–Shkoller [41] proposed the "variational integrator" based on the variational principal. Its name is close to the discrete variational derivative method, but their methods are quite different. Marsden–West [42] is a good review of them. Bridges–Reich [6] developed another interesting method, "the multi-symplectic method", for Hamiltonian partial differential equations. They transformed the original equations to the multi-symplectic form and designed some numerical schemes based on the form. Please refer to [10, 29, 30] for the method. Finally, we introduce other excellent reviews including Leimkuhler–Reich [37] and Lubich [39] for the reader who is interested in the structure-preserving methods.

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