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Finite Difference Schemes for $\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{\alpha} \frac{\delta G}{\delta u}$ That Inherit Energy Conservation or Dissipation Property[1]

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We propose a new procedure for designing by rote finite difference schemes that inherit energy conservation or dissipation property from nonlinear partial differential equations, such as the Korteweg–de Vries (KdV) equation and the Cahn–Hilliard equation. The most important feature of our procedure is a rigorous discretization of variational derivatives using summation by parts, which implies that the inherited properties are satisfied exactly. Since the inherited properties are kept even if the time mesh size changes in the time-evolution process, we can use some appropriate time mesh adaptive methods to obtain numerical solutions through the derived schemes. Because of these properties the derived schemes are expected to be numerically stable and yield solutions converging to PDE solutions and sufficiently flexible to treat. The inheritance of the energy conservation and dissipation properties are verified numerically for the KdV equation and the Cahn–Hilliard equation

Key Words: finite difference method; energy conservation; energy dissipation; mass conservation; Korteweg–de Vries equation; Cahn–Hilliard equation.

1. INTRODUCTION

We consider finite difference schemes that inherit energy conservation or dissipation property from nonlinear partial differential equations.

The study of schemes with conservation property was initiated by Courant *et al.* [5]. This so-called "energy method" attracted widespread attention in 1950s, as documented by Richtmyer and Morton [28, Section 6]. This method was primarily studied to prove the stability, existence, and uniqueness of solutions of schemes. The main emphasis was on stability rather than conservation property.

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Since 1970s the main interest has shifted from stability to the conservation property itself. Studies placing greater emphasis on the conservation property include those by Strauss and Vazquez [31], Greenspan [19], Li and Vu-Quoc [24], French [10, 11], Fla [9], Nicolaides [26], McLachlan [25], and Hyman [22]. For energy conservation, Strauss and Vazquez [31] discussed schemes for the linear Klein–Gordon equation, Greenspan [19] for the initial value problem $\ddot{x} = f(x)$, and Li and Vu-Quoc [24] for the nonlinear Klein–Gordon equation. Fla [9] showed schemes that inherit energy conservation property and mass conservation property from DNLS (derivative nonlinear Schrödinger) equation. French [10, 11] proposed some generic FEM schemes that preserve the energy properties of nonlinear PDEs. A control volume method for overcoming the difficulty of discretizing the div-curl system is proposed in Nicolaides [26]. McLachlan [25] presents an algebraic method for the construction of numerical schemes that inherit some symmetries of solutions of ODE. The "mimetic method" shown in Hyman [22] mimics the fundamental properties of a system using discrete operators that consist of discretized laws of vector and tensor calculus. The famous "symplectic method" [30], applicable to Hamilton systems, may be regarded as one application based on this formulation. In their recent paper [24], Li and Vu-Quoc, describe this shift in emphasis, noting that "in some areas, the ability to preserve some invariant properties of the original differential equation is a criterion to judge the success of a numerical simulation." This shift and recent works may be considered "geometric integration" studies [2].

Still this formulation has been restricted to (the case of) conservative systems, treating only invariants as the characteristic properties to inherit. Since the dissipation laws are as essential as the conservation laws for some problems such as the spinodal decomposition problem [3] we must treat the dissipation laws as another fundamental property to inherit. Through considering this spinodal decomposition problem we succeeded in proposing a new finite difference scheme that inherits the energy dissipation property from the Cahn–Hilliard equation in [16]. Du and Nicolaides [6] also proposed interesting FEM and FDM schemes that inherit the energy dissipation property for the equation under Dirichlet boundary conditions. These results also exploit possibility of unification of the conservation laws and the dissipation laws as the characteristic properties to inherit.

In this paper, defining some discrete mathematical notions in a rigorous manner we show a unified formulation for designing by rote finite difference schemes that inherit the conservation property or the dissipation property. The family of equations that we consider in this paper is

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{\alpha} \frac{\delta G}{\delta u}, \qquad \alpha = 0, 1, 2, 3, \ldots, \tag{1}$$

where $G = G(u, u_x)$ is a function of both u and $u_x = \frac{\partial u}{\partial x}$, and $\frac{\delta G}{\delta u}$ is a variational derivative of function $G(u, u_x)$ for u. Boundary conditions, properties of this family, the definition of G, etc., are described in Section 2. When α is odd, the property of the equations to be inherited by the schemes is $\frac{\partial}{\partial t}\int G\,dx = 0$ and is called the "energy conservation property" in this paper. When α is even, it is $(-1)^{\alpha/2+1}\frac{\partial}{\partial t}\int G\,dx \leq 0$ and called the "energy dissipation property." Under certain conditions the "mass conservation property," $\frac{\partial}{\partial t}\int u(x,t)\,dx = 0$, is inherited in addition. Now the question is whether we can design a finite difference scheme that inherits the above properties for Eq. (1). We answer this question in the affirmative by making discrete replicas of the cause-and-effect relationship between Eq. (1) and the above properties in the context of exact finite difference calculus such as the summation-by-parts, which corresponds to the integral-by-parts. This idea is quite natural but there has been no study that states a concrete and general-purpose method without vagueness. In order to eliminate vagueness we define some discrete mathematical notions strictly. The most essential notion is a discrete variational derivative under finite summation. Hirota [21] mentioned a similar notion, the discrete Euler derivative, obtained heuristically for some special examples. The basic idea of this formulation has been reported in [14, 15] without precise mathematical discussion. Concerning the derived schemes themselves, we can use appropriate time mesh adaptive methods because the discrete replicas of the cause-and-effect relationship are local with respect to time step. Because of this property we can expect that the derived schemes are sufficiently flexible to treat, in addition to being stable and convergent.

The contents of this paper are as follows. In Section 2 we describe the "target" equations and the characteristic properties precisely. The cause-and-effect relationship between the target equations and the inherited properties is shown in the continuous context. In Section 3 definitions and properties of discrete operators are shown. In Section 4 we show the schemes designed to inherit the above properties. In Sections 4.2 and 4.3 we prove that derived schemes inherit the above properties. The proof is the form of the discrete cause-and-effect relationship between the target equations and the inherited properties in the context of finite difference calculus. In Section 5 we show schemes and numerical solutions for some example equations, the Korteweg–de Vries equation, a linear diffusion equation, and the Cahn–Hilliard equation. We show that the derived schemes have some good features. We conclude with a summary of the results in this paper.

2. EQUATIONS AND PROPERTIES

The purpose of this section is to describe equations and their characteristic properties, which we consider. The relationship between an equation and its properties, described in this section, is fundamental to this paper.

For $\alpha = 0, 1, 2, 3, \ldots$ we consider the following equation in function $u(x, t)$,

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{\alpha} \frac{\delta G}{\delta u}, \tag{2}$$

where $x \in \Omega = [0, L]$, $L < \infty$, is the one-dimensional space variable and t is the time variable. Function $G = G(u, u_x)$ is called the "energy function" in this paper since it often corresponds to a local free energy function in physical applications. $\frac{\delta G}{\delta u}$ is a variational derivative of the function G for u and is calculated as $\frac{\delta G}{\delta u} = \frac{\partial G}{\partial u} - \frac{d}{dx}(\frac{\partial G}{\partial u_x})$.

We consider a class of boundary conditions that satisfy the following two assumptions. The first assumption is

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_{x=0}^{L} = 0, \tag{3}$$

which is satisfied, e.g., by the Dirichlet b.c. or the natural b.c. or the periodical b.c. The second one is

$$\left[\sum_{l=1}^{\alpha/2}(-1)^{l-1}F^{(l-1)}F^{(\alpha-l)}\right]_{x=0}^{L} = 0: \qquad \alpha \text{ is even}$$

$$\left[\sum_{l=1}^{(\alpha-1)/2}(-1)^{l-1}F^{(l-1)}F^{(\alpha-l)} + \frac{1}{2}(-1)^{(\alpha-1)/2}F^{((\alpha-1)/2)}F^{((\alpha-1)/2)}\right]_{x=0}^{L} = 0: \qquad \alpha \text{ is odd,} \tag{4}$$

where $F^{(l)} \stackrel{\text{def}}{=} (\frac{\partial}{\partial x})^l \frac{\delta G}{\delta u}$ and summations in (4) are defined as 0 when the upper limit of the running index is less than the lower limit. This convention applies to all summations in this paper.

For the solution $u(x,t)$ of (2) under boundary conditions that satisfy two assumptions (3) and (4), time dependency of the integral of the energy function is indicated as

$$\begin{aligned}
&\frac{d}{dt}\int_0^L G(u,u_x)\,dx \\
&\quad = \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\,dx + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_{x=0}^{L} \\
&\quad = \int_0^L \frac{\delta G}{\delta u}\left(\frac{\partial}{\partial x}\right)^{\alpha}\frac{\delta G}{\delta u}\,dx \\
&\quad = \text{LHS(4)} + \delta(\alpha)(-1)^{\alpha/2}\int_0^L \left\{\left(\frac{\partial}{\partial x}\right)^{\alpha/2}\frac{\delta G}{\delta u}\right\}^2 dx \\
&\quad = \begin{cases} (-1)^{\alpha/2}\cdot(\text{Nonnegative}) & (\text{Dissipative}): \quad \alpha \text{ is even} \\ 0 & (\text{Conservative}): \quad \alpha \text{ is odd,} \end{cases}
\end{aligned} \tag{5}$$

where

$$\delta(\alpha) \stackrel{\text{def}}{=} \begin{cases} 1: & \alpha \text{ is even} \\ 0: & \alpha \text{ is odd.} \end{cases} \tag{6}$$

We call this the "energy dissipation property" when α is even and the "energy conservation property" when α is odd. Note that Eq. (5) is the most fundamental continuous equation in this paper since it describes the cause-and-effect relationship between equations and properties. If the condition

$$\begin{aligned}
\int_0^L \frac{\delta G}{\delta u}\,dx = 0: &\qquad \alpha = 0 \\
\left[\left(\frac{\partial}{\partial x}\right)^{\alpha-1}\frac{\delta G}{\delta u}\right]_{x=0}^{L} = 0: &\qquad \alpha > 0
\end{aligned} \tag{7}$$

is satisfied in addition to conditions (3) and (4), the time dependency of integral of $u(x,t)$

is

$$\frac{d}{dt}\int_0^L u(x,t)\,dx = \int_0^L \frac{\partial u}{\partial t}\,dx = \int_0^L \left(\frac{\partial}{\partial x}\right)^{\alpha}\frac{\delta G}{\delta u}\,dx$$
$$= \begin{cases} \int_0^L \frac{\delta G}{\delta u}\,dx = 0: & \alpha = 0 \\ \left[\left(\frac{\partial}{\partial x}\right)^{\alpha-1}\frac{\delta G}{\delta u}\right]_{x=0}^{L} = 0: & \alpha > 0. \end{cases} \tag{8}$$

We call this property the "mass conservation property." We call Eq. (2) "the dissipation problem" where α is even and (3) and (4) (and (7)) are satisfied. We call Eq. (2) "the conservation problem" where α is odd and (3) and (4) (and (7)) are satisfied.

For example, the linear convection equation

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \tag{9}$$

and the Korteweg–de Vries equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{2}u^2 + \frac{\partial^2 u}{\partial x^2}\right) \tag{10}$$

are conservation problems. A linear diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \tag{11}$$

the prominence temperature equation [1, pp. 7, 8]

$$\frac{\partial u}{\partial t} = \frac{\partial^2\left(u^{7/2}\right)}{\partial x^2}, \tag{12}$$

and the Cahn–Hilliard equation [3]

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right), \qquad p < 0,\ q < 0,\ r > 0, \tag{13}$$

are dissipation problems.

As described in the Introduction, our main interest in this paper is to discretize the derivation process (5) of the dissipation/conservation property. For this, all operations and calculus, i.e., differential, integral, integral by parts, and variational derivative, in Eq. (5) must be discretized consistently. We choose one consistent "set" of discrete operators carefully for this purpose and describe these operators in Section 3.

3. DISCRETE SYMBOLS

In this section we introduce a consistent set of discrete operators.

3.1. *Symbol Definitions*

We suppose that the space mesh size is uniform. We define shift operators $s_k^+, s_k^-, s_k^{\langle 1\rangle}, \ldots,$

$$s_k^{\langle 0\rangle} \stackrel{\text{def}}{=} 1, \tag{14}$$

$$s_k^+ f_k \stackrel{\text{def}}{=} f_{k+1}, \tag{15}$$

$$s_k^- f_k \stackrel{\text{def}}{=} f_{k-1}, \tag{16}$$

$$s_k^{\langle 1 \rangle} \stackrel{\text{def}}{=} \frac{s_k^+ + s_k^-}{2}. \tag{17}$$

We define δ_k^+, δ_k^- and the nth difference operator $\delta_k^{\langle n \rangle}$, which is a discretization of the nth differential operator, as

$$\delta_k^{\langle 0 \rangle} \stackrel{\text{def}}{=} 1, \tag{18}$$

$$\delta_k^+ \stackrel{\text{def}}{=} \frac{s_k^+ - 1}{\Delta x}, \tag{19}$$

$$\delta_k^- \stackrel{\text{def}}{=} \frac{1 - s_k^-}{\Delta x}, \tag{20}$$

$$\delta_k^{\langle 1 \rangle} \stackrel{\text{def}}{=} \frac{s_k^+ - s_k^-}{2\Delta x}, \tag{21}$$

$$\delta_k^{\langle 2 \rangle} \stackrel{\text{def}}{=} \frac{s_k^+ - 2 + s_k^-}{\Delta x^2}, \tag{22}$$

$$\delta_k^{\langle 2m+1 \rangle} \stackrel{\text{def}}{=} \delta_k^{\langle 1 \rangle} \delta_k^{\langle 2m \rangle}, \qquad m \geq 1, \tag{23}$$

$$\delta_k^{\langle 2m+2 \rangle} \stackrel{\text{def}}{=} \delta_k^{\langle 2 \rangle} \delta_k^{\langle 2m \rangle}, \qquad m \geq 1. \tag{24}$$

We adopt these difference operators for the following reasons:

- operators should be "symmetric" (i.e., they should not vary when $\Delta x \to -\Delta x$);
- the number of reference points of the nth difference operator should be $n + 1$ (this number is minimum to approximate the differential operator);
- the discrepancy between difference operator and differential operator should be minimum under the above conditions.

We also define averaging operators μ_k^+, μ_k^-, $\mu_k^{\langle 0 \rangle}$, $\mu_k^{\langle 1 \rangle}$, $\ldots$, as

$$\mu_k^{\langle 0 \rangle} \stackrel{\text{def}}{=} 1, \tag{25}$$

$$\mu_k^+ \stackrel{\text{def}}{=} \frac{1 + s_k^+}{2}, \tag{26}$$

$$\mu_k^- \stackrel{\text{def}}{=} \frac{1 + s_k^-}{2}, \tag{27}$$

$$\mu_k^{\langle 1 \rangle} \stackrel{\text{def}}{=} \frac{\mu_k^+ + \mu_k^-}{2} = \frac{1 + s_k^{\langle 1 \rangle}}{2}. \tag{28}$$

As a discretization of the integral we adopt the summation $\sum''$, which is defined by

$$\sum_{k=0}^{N}{}'' f_k \Delta x \stackrel{\text{def}}{=} \left(\frac{1}{2} f_0 + \sum_{k=1}^{N-1} f_k + \frac{1}{2} f_N \right) \Delta x \tag{29}$$

for the same reasons as above.

3.2. *Discrete Calculus*

Some relationships between difference operators and summations are described in this subsection.

First, we describe the inverse relationship between difference operators and summation operators for any $h > 0$, $h \in \mathbf{N}$,

$$\sum_{k=0}^{N}{}'' \, \delta_k^{\langle h \rangle} f_k \Delta x = \left[\mu_k^{\langle \sigma(h) \rangle} \delta_k^{\langle h-1 \rangle} f_k \right]_{k=0}^{N} \tag{30}$$

$$\delta_k^{\langle h \rangle} \sum_{l=0}^{k}{}'' \, f_l \Delta x = \mu_k^{\langle \sigma(h) \rangle} \delta_k^{\langle h-1 \rangle} f_k, \tag{31}$$

where

$$[f_k]_{k=0}^{N} \stackrel{\text{def}}{=} f_N - f_0, \tag{32}$$

$$\sigma(h) \stackrel{\text{def}}{=} h \bmod 2 = \begin{cases} 0: & h \text{ is even} \\ 1: & h \text{ is odd.} \end{cases} \tag{33}$$

The following relationship is "summation by parts," which corresponds to integration by parts:

$$\sum_{k=0}^{N}{}'' \, f_k(\delta_k^+ g_k) \, \Delta x + \sum_{k=0}^{N}{}'' \, (\delta_k^- f_k) g_k \Delta x = \left[\frac{f_k(s_k^+ g_k) + (s_k^- f_k) g_k}{2} \right]_{k=0}^{N}. \tag{34}$$

Repeated application of the summation by parts yields

$$\sum_{k=0}^{N}{}'' \, f_k \delta_k^{\langle h \rangle} f_k \Delta x$$

$$= \begin{cases} (-1)^{h/2} \sum_{k=0}^{\prime\prime N} \hat{F}_k^{\langle h/2, h \rangle} \Delta x \\ \quad + \Bigg[\sum_{\substack{1 \le l \le h/2 \\ l:\ \text{even}}} (-1) \dfrac{2\hat{F}_k^{\langle l-1 \rangle} \hat{F}_k^{\langle h-l \rangle} + \left(\delta_k^+ \hat{F}_k^{\langle l-2 \rangle}\right)\left(s_k^+ \hat{F}_k^{\langle h-l \rangle}\right) + \left(\delta_k^- \hat{F}_k^{\langle l-2 \rangle}\right)\left(s_k^- \hat{F}_k^{\langle h-l \rangle}\right)}{4} \\ \quad + \sum_{\substack{1 \le l \le h/2 \\ l:\ \text{odd}}} \dfrac{2\hat{F}_k^{\langle l-1 \rangle} \hat{F}_k^{\langle h-l \rangle} + \left(s_k^+ \hat{F}_k^{\langle l-2 \rangle}\right)\left(\delta_k^+ \hat{F}_k^{\langle h-l \rangle}\right) + \left(s_k^- \hat{F}_k^{\langle l-2 \rangle}\right)\left(\delta_k^- \hat{F}_k^{\langle h-l \rangle}\right)}{4} \Bigg]_{k=0}^{N} : & h \text{ is even} \\ \Bigg[\sum_{\substack{1 \le l \le (h-1)/2 \\ l:\ \text{even}}} (-1) \dfrac{\left(\delta_k^+ \hat{F}_k^{\langle l-2 \rangle}\right)\left(\delta_k^+ \hat{F}_k^{\langle h-l-1 \rangle}\right) + \left(\delta_k^- \hat{F}_k^{\langle l-2 \rangle}\right)\left(\delta_k^- \hat{F}_k^{\langle h-l-1 \rangle}\right)}{2} \\ \quad + \sum_{\substack{1 \le l \le (h-1)/2 \\ l:\ \text{odd}}} \dfrac{\hat{F}_k^{\langle l-1 \rangle}\left(s_k^{\langle 1 \rangle} \hat{F}_k^{\langle h-l \rangle}\right) + \left(s_k^{\langle 1 \rangle} \hat{F}_k^{\langle l-1 \rangle}\right) \hat{F}_k^{\langle h-l \rangle}}{2} \\ \quad + \frac{1}{2}(-1)^{(h-1)/2} \hat{F}_k^{\langle (h-1)/2, h \rangle} \Bigg]_{k=0}^{N} : & h \text{ is odd,} \end{cases} \tag{35}$$

where $h \in \mathbf{N}^+$,

$$\hat{F}_k^{\langle l \rangle} \stackrel{\text{def}}{=} \delta_k^{\langle l \rangle} f_k, \tag{36}$$

$$\hat{F}_k^{\langle l, l' \rangle} \stackrel{\text{def}}{=} \begin{cases} \hat{F}_k^{\langle l \rangle} \left(s_k^{\langle \sigma(l') \rangle} \hat{F}_k^{\langle l \rangle} \right) : & l \text{ is even} \\ \dfrac{\left(\delta_k^+ \hat{F}_k^{\langle l-1 \rangle}\right)^2 + \left(\delta_k^- \hat{F}_k^{\langle l-1 \rangle}\right)^2}{2} : & l \text{ is odd} \end{cases} \tag{37}$$

for $l, l' \in \mathbf{N}$. The derivation of (35) is shown in the Appendix.

3.3. *Discrete Variational Derivative*

In this subsection we describe the definition and properties of the discrete variational derivative, which is derived from the definitions in Section 3.1 using relations in Section 3.2.

First we assume that a "discrete energy function" $G_{\mathrm{d}}(U) = (G_{\mathrm{d}}(U)_k)_{k\in\mathbf{Z}}$ where $U = (U_k)_{k\in\mathbf{Z}}$, which is given as an approximation to $G(u, u_x)$, takes the form

$$G_{\mathrm{d}}(U)_k = \sum_{l=1}^{m} f_l(U_k) g_l^{+}(\delta_k^{+} U_k) g_l^{-}(\delta_k^{-} U_k), \qquad k \in \mathbf{Z}, \tag{38}$$

where $m \in \mathbf{N}^{+}$ and $f_l, g_l^{+}, g_l^{-} : \mathbf{R} \to \mathbf{R}$ are differentiable functions. U_k is intended to be an approximation to $u(k\Delta x)$. For such G_{d} we define the discrete variational derivative

$$\frac{\delta G_{\mathrm{d}}}{\delta(U, V)} = \left(\left(\frac{\delta G_{\mathrm{d}}}{\delta(U, V)}\right)_k\right)_{k\in\mathbf{Z}}$$

of G_{d} for (U, V) as

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(U, V)}\right)_k \stackrel{\mathrm{def}}{=} \sum_{l=1}^{m} \left(\frac{d f_l}{d(U_k, V_k)} \frac{g_l^{+}(\delta_k^{+} U_k) g_l^{-}(\delta_k^{-} U_k) + g_l^{+}(\delta_k^{+} V_k) g_l^{-}(\delta_k^{-} V_k)}{2} - \delta_k^{+} W_l^{-}(U, V)_k - \delta_k^{-} W_l^{+}(U, V)_k \right), \tag{39}$$

where $U = (U_k)_{k\in\mathbf{Z}}$, $V = (V_k)_{k\in\mathbf{Z}}$, and

$$W_l^{+}(U, V)_k = \left(\frac{f_l(U_k) + f_l(V_k)}{2}\right)\left(\frac{g_l^{-}(\delta_k^{-} U_k) + g_l^{-}(\delta_k^{-} V_k)}{2}\right) \frac{d g_l^{+}}{d(\delta_k^{+} U_k, \delta_k^{+} V_k)} \tag{40}$$

$$W_l^{-}(U, V)_k = \left(\frac{f_l(U_k) + f_l(V_k)}{2}\right)\left(\frac{g_l^{+}(\delta_k^{+} U_k) + g_l^{+}(\delta_k^{+} V_k)}{2}\right) \frac{d g_l^{-}}{d(\delta_k^{-} U_k, \delta_k^{-} V_k)} \tag{41}$$

$$\frac{df}{d(a, b)} \stackrel{\mathrm{def}}{=} \begin{cases} \frac{f(a) - f(b)}{a-b} : & a \neq b \\ \frac{df}{da} : & a = b. \end{cases} \tag{42}$$

We note that this definition is well defined.

The above definition of the discrete variational derivative parallels the definition of $\frac{\delta G}{\delta u}$. First recall that when $u \cong v$ the variational derivative satisfies (by definition)

$$J[u] - J[v] \cong \int_{\Omega} \frac{\delta G}{\delta u}(u - v)\, dx + \left[\frac{\partial G}{\partial u_x}(u - v)\right]_{\partial\Omega}, \tag{43}$$

where

$$J[u] \stackrel{\mathrm{def}}{=} \int_{\Omega} G(u)\, dx. \tag{44}$$

Consider a discrete functional $J_{\mathrm{d}}[U]$ defined as

$$J_{\mathrm{d}}[U] = \sum_{k=0}^{N}{}'' G_{\mathrm{d}}(U)_k \Delta x. \tag{45}$$

By the summation-by-parts (34) applied to the difference $J_{\mathrm{d}}[U] - J_{\mathrm{d}}[V]$ we obtain

$$\begin{aligned} J_{\mathrm{d}}[U] - J_{\mathrm{d}}[V] &= \sum_{k=0}^{N}{}'' \left\{ \sum_{l=1}^{m} \left(\frac{d f_l}{d(U_k, V_k)} \frac{g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k) + g_l^+(\delta_k^+ V_k) g_l^-(\delta_k^- V_k)}{2} \right.\right. \\ &\quad \left.\left. - \delta_k^+ W_l^-(U,V)_k - \delta_k^- W_l^+(U,V)_k \right) \right\} (U_k - V_k) \Delta x \\ &\quad + \left[\frac{1}{2} \sum_{l=1}^{m} (W_l^+(U,V)_k s_k^+(U_k - V_k) + W_l^-(U,V)_k s_k^-(U_k - V_k) \right. \\ &\quad \left. + (s_k^+ W_l^-(U,V)_k + s_k^- W_l^+(U,V)_k)(U_k - V_k)) \right]_{k=0}^{N} \\ &= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(U,V)_k} (U_k - V_k) \Delta x + \left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U,V)_k \right]_{k=0}^{N}, \end{aligned} \tag{46}$$

where

$$\begin{aligned} \frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U,V)_k \stackrel{\mathrm{def}}{=} & \frac{1}{2} \sum_{l=1}^{m} (W_l^+(U,V)_k s_k^+(U_k - V_k) + W_l^-(U,V)_k s_k^-(U_k - V_k) \\ & + (s_k^+ W_l^-(U,V)_k + s_k^- W_l^+(U,V)_k)(U_k - V_k)). \end{aligned} \tag{47}$$

This yields

$$J_{\mathrm{d}}[U] - J_{\mathrm{d}}[V] = \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(U,V)_k} (U_k - V_k) \Delta x \tag{48}$$

if

$$\left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U,V)_k \right]_{k=0}^{N} = 0.$$

Equation (46) may be regarded as a discrete analogue of (43).

Remark. In the more general case where G involves u_{xx}, u_{xxx}, etc., the discrete variational derivative of G can be treated in a similar manner, as will be reported soon elsewhere.

4. DESIGN OF SCHEMES

In this section we show the finite difference scheme that we propose. $U_k^{(n)}$ means the approximation of $u(k\Delta x, n\Delta t)$ in this section. Figure 1 shows the proposed design procedure for obtaining finite difference schemes.

Recall our assumption on the discretization of the energy function G that G_{d} must be in the form (38). This is because we use the discrete variational derivative of G_{d}.

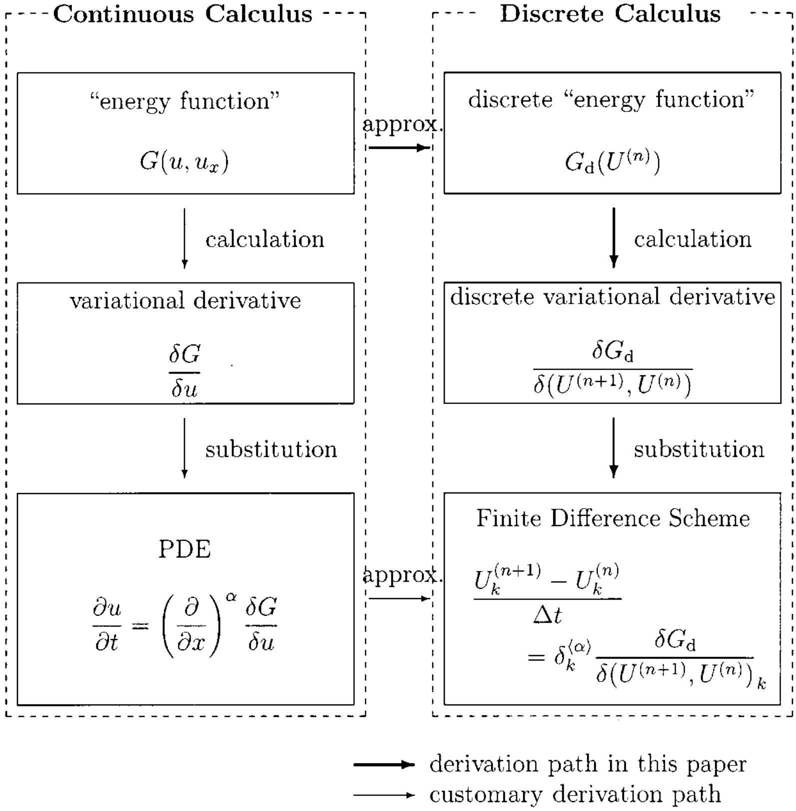

FIG. 1. Design flowchart of the finite difference scheme.

4.1. *The Finite Difference Method*

For the equation

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{\alpha} \frac{\delta G}{\delta u}$$

in (2) with $\alpha \in \mathbf{N}$, we propose the finite difference scheme

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle\alpha\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k}, \qquad 0 \le k \le N,\ k \in \mathbf{Z},\ n \in \mathbf{N}, \tag{49}$$

with discrete boundary conditions. We note that the proposed scheme (49) involves $(U_k^{(n+1)})_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ and $(U_k^{(n)})_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ where $(a_k)_{k=m_1}^{m_2} \stackrel{\text{def}}{=} \{a_{m_1}, a_{m_1+1}, a_{m_1+2}, \ldots, a_{m_2}\}$,

$$\alpha'' \stackrel{\text{def}}{=} \left\lceil \frac{\alpha}{2} \right\rceil, \tag{50}$$

and

$$\beta = \beta(G_{\rm d}) \overset{\rm def}{=} \begin{cases} 0: & g_l^+ = \text{const. and } g_l^- = \text{const. for } 1 \le {}^\forall l \le m \\ 1: & \text{not in above case and } g_l^+ = \text{const. or } g_l^- = \text{const. for } 1 \le {}^\forall l \le m \\ 2: & \text{otherwise.} \end{cases} \tag{51}$$

The discrete boundary conditions may be arbitrary under the following two constraints.

The first constraint. $(U_k^{(n+1)})_{k=-\alpha''-\beta}^{-1}$ and $(U_k^{(n+1)})_{k=N+1}^{N+\alpha''+\beta}$ must be described explicitly with $(U_k^{(n)})_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ and $(U_k^{(n+1)})_{k=0}^{N}$ through the discrete boundary conditions. This also implies that $(U_k^{(0)})_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ are given. This constraint is necessary to make the proposed scheme (49) consistent.

The second constraint. This corresponds to (3), (4) in the continuous context. The first condition, which corresponds to (3), is

$$\left[\frac{\partial G_{\rm d}}{\partial \delta U}\big(U^{(n+1)}, U^{(n)}\big)_k\right]_{k=0}^{N} = 0. \tag{52}$$

The second one, which corresponds to (4), is

$$\begin{cases}
\left[\sum_{\substack{1\le l\le \alpha/2\\ l:\ \text{even}}} (-1)\frac{2\tilde F_k^{\langle l-1\rangle}\tilde F_k^{\langle \alpha-l\rangle} + \big(\delta_k^+\tilde F_k^{\langle l-2\rangle}\big)\big(s_k^+\tilde F_k^{\langle \alpha-l\rangle}\big) + \big(\delta_k^-\tilde F_k^{\langle l-2\rangle}\big)\big(s_k^-\tilde F_k^{\langle \alpha-l\rangle}\big)}{4} \right. \\
\left. + \sum_{\substack{1\le l\le \alpha/2\\ l:\ \text{odd}}} \frac{2\tilde F_k^{\langle l-1\rangle}\tilde F_k^{\langle \alpha-l\rangle} + \big(s_k^+\tilde F_k^{\langle l-2\rangle}\big)\big(\delta_k^+\tilde F_k^{\langle \alpha-l\rangle}\big) + \big(s_k^-\tilde F_k^{\langle l-2\rangle}\big)\big(\delta_k^-\tilde F_k^{\langle \alpha-l\rangle}\big)}{4}\right]_{k=0}^{N} = 0: \quad \alpha \text{ is even} \\
\left[\sum_{\substack{1\le l\le (\alpha-1)/2\\ l:\ \text{even}}} (-1)\frac{\big(\delta_k^+\tilde F_k^{\langle l-2\rangle}\big)\big(\delta_k^+\tilde F_k^{\langle \alpha-l-1\rangle}\big) + \big(\delta_k^-\tilde F_k^{\langle l-2\rangle}\big)\big(\delta_k^-\tilde F_k^{\langle \alpha-l-1\rangle}\big)}{2} \right. \\
+ \sum_{\substack{1\le l\le (\alpha-1)/2\\ l:\ \text{odd}}} \frac{\tilde F_k^{\langle l-1\rangle}\big(s_k^{\langle 1\rangle}\tilde F_k^{\langle \alpha-l\rangle}\big) + \big(s_k^{\langle 1\rangle}\tilde F_k^{\langle l-1\rangle}\big)\tilde F_k^{\langle \alpha-l\rangle}}{2} \\
\left. + \frac{1}{2}(-1)^{(\alpha-1)/2}\tilde F_k^{\langle (\alpha-1)/2,\alpha\rangle}\right]_{k=0}^{N} = 0: \quad \alpha \text{ is odd,}
\end{cases} \tag{53}$$

where

$$\tilde F_k^{\langle l\rangle} \overset{\rm def}{=} \delta_k^{\langle l\rangle}\frac{\delta G_{\rm d}}{\delta\big(U^{(n+1)}, U^{(n)}\big)_k}, \tag{54}$$

$$\tilde F_k^{\langle l,l'\rangle} \overset{\rm def}{=} \begin{cases} \tilde F_k^{\langle l\rangle}\big(s_k^{\langle \sigma(l')\rangle}\tilde F_k^{\langle l\rangle}\big): & l \text{ is even} \\ \dfrac{\big(\delta_k^+\tilde F_k^{\langle l-1\rangle}\big)^2 + \big(\delta_k^-\tilde F_k^{\langle l-1\rangle}\big)^2}{2}: & l \text{ is odd.} \end{cases} \tag{55}$$

When the original boundary conditions satisfy (7), the discrete boundary condition should also satisfy

$$\begin{aligned} \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} \Delta x = 0 : \qquad & \alpha = 0 \\ \left[\mu_k^{\langle\sigma(\alpha)\rangle} \delta_k^{\langle\alpha-1\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k}\right]_{k=0}^{N} = 0 : \qquad & \alpha > 0. \end{aligned} \tag{56}$$

4.2. *Properties of the Scheme for the Conservation Problem*

In this subsection we describe properties of the derived scheme for the conservation problem (2) with odd α.

THEOREM 4.1 (Energy Conservation). *Let $U_k^{(n)}$ be computed through* (49), (52), *and* (53) *for odd α. Then the total energy $\sum''^{N}_{k=0} G_{\mathrm{d}}(U^{(n)})_k \Delta x$ is independent of time step n.*

Proof.

$$\begin{aligned} &\frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(U^{(n+1)}\right)_k \Delta x - \sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(U^{(n)}\right)_k \Delta x\right\} \\ &= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k}\left(\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t}\right)\Delta x \\ &= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} \cdot \delta_k^{\langle\alpha\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} \Delta x \\ &= \mathrm{LHS}(53) \\ &= 0. \end{aligned} \tag{57}$$

The first equality is derived from (48) and (52), the second is from the scheme (49), the third is from (35), and the last is from (53). ■

THEOREM 4.2 (Mass Conservation). *Let $U_k^{(n)}$ be computed through* (49), (52), *and* (53) *for odd α. If the optional condition* (56) *is satisfied by $U_k^{(n)}$, then the total mass $\sum''^{N}_{k=0} U_k^{(n)} \Delta x$ is independent of time step n.*

Proof.

$$\begin{aligned} \frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' U_k^{(n+1)} \Delta x - \sum_{k=0}^{N}{}'' U_k^{(n)} \Delta x\right\} &= \sum_{k=0}^{N}{}'' \delta_k^{\langle\alpha\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} \Delta x \\ &= \left[\mu_k^{\langle 1\rangle} \delta_k^{\langle\alpha-1\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k}\right]_{k=0}^{N} \\ &= 0. \end{aligned} \tag{58}$$

The first equality is derived from the scheme (49), the second is from (30), and the last is from the optional condition (56). ■

Remark. Looking at these proofs, we find that we can change the time mesh size Δt with respect to time step n as Δt_n, still preserving the above theorems. This means that we can use some appropriate time mesh adaptive methods to obtain numerical solutions through the proposed scheme (49). For some severe problems, this property may be essentially helpful. This state is also valid for the dissipative problem in the following subsection.

4.3. *Properties of the Scheme for the Dissipative Problem*

In this subsection we describe properties of the derived scheme for the dissipative problem (2) with even α.

THEOREM 4.3 (Energy Dissipation). *Let $U_k^{(n)}$ be computed through* (49), (52), *and* (53) *for even α. Then the* (*sign-modified*) *total energy* $(-1)^{\alpha/2+1}\sum_{k=0}^{N}{}'' G_{\mathrm{d}}(U^{(n)})_k \Delta x$ *decreases as the time step n increases.*

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' G_{\mathrm{d}}\big(U^{(n+1)}\big)_k \Delta x - \sum_{k=0}^{N}{}'' G_{\mathrm{d}}\big(U^{(n)}\big)_k \Delta x\right\} \\
&= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\big(U^{(n+1)}, U^{(n)}\big)_k}\left(\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t}\right)\Delta x \\
&= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta\big(U^{(n+1)}, U^{(n)}\big)_k} \cdot \delta_k^{\langle\alpha\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\big(U^{(n+1)}, U^{(n)}\big)_k} \Delta x \\
&= \mathrm{LHS}(53) + (-1)^{\alpha/2} \sum_{k=0}^{N}{}'' \tilde{F}_k^{\langle \alpha/2, \alpha\rangle} \Delta x \\
&= (-1)^{\alpha/2} \cdot (\text{Nonnegative}),
\end{aligned} \tag{59}$$

where $\tilde{F}_k^{\langle l\rangle}$ is defined in (54). The first equality is derived from (48) and (52), the second is from the scheme (49), the third is from (35), and the last is from (53). ∎

THEOREM 4.4 (Mass Conservation). *Let $U_k^{(n)}$ be computed through* (49), (52), *and* (53) *for even α. If the optional condition* (56) *is satisfied by $U_k^{(n)}$, then the total mass* $\sum_{k=0}^{N}{}'' U_k^{(n)} \Delta x$ *is independent of time step n.*

Proof.

$$\begin{aligned}
\frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' U_k^{(n+1)}\Delta x - \sum_{k=0}^{N}{}'' U_k^{(n)}\Delta x\right\} &= \sum_{k=0}^{N}{}'' \delta_k^{\langle\alpha\rangle} \frac{\delta G_{\mathrm{d}}}{\delta\big(U^{(n+1)}, U^{(n)}\big)_k}\Delta x \\
&= \begin{cases} \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})} \Delta x : & \alpha = 0 \\ \left[\delta_k^{\langle \alpha-1\rangle} \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k}\right]_{k=0}^{N} : & \alpha > 0 \end{cases} \\
&= 0.
\end{aligned} \tag{60}$$

The first equality is derived from the scheme (49), the second is from (30), and the last is from the optional condition (56). ∎

Remark. As described in the above remark, we can also change the time mesh size Δt with respect to time step n as Δt_n, still preserving the above theorems.

5. APPLICATIONS

Some examples using the proposed method are shown in this section.

5.1. *The Korteweg–de Vries Equation*

We consider the Korteweg–de Vries equation as an example for $\alpha = 1$ in (2). This is a well-known nonlinear equation which has soliton solutions. Numerical solution of this equation is relatively difficult and studies through the finite difference method are [12, 17, 18, 20, 27, 29, 34]. It has been proven that some schemes are unconditionally stable; see, for instance, [23] and [33]. The equation is

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{1}{2}u^2 + \frac{\partial^2 u}{\partial x^2}\right\} \tag{61}$$

and the periodic condition

$$u(x + nL) = u(x), \qquad n \in \mathbf{Z}, \tag{62}$$

is imposed.

The KdV equation is an instance of (2) with $\alpha = 1$ and

$$G(u, u_x) = \frac{1}{6}u^3 - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2, \tag{63}$$

and the condition (62) satisfies (3) and (4). For this system the total energy is conserved, i.e.,

$$\frac{d}{dt}\int_0^L G(u, u_x)\,dx = 0. \tag{64}$$

Since the periodic condition satisfies (7), the total mass is also conserved, i.e.,

$$\frac{d}{dt}\int_0^L u(x, t)\,dx = 0. \tag{65}$$

According to Section 4, we obtain the scheme for this equation. First, we discretize "energy function" $G(u, u_x)$ of (63) to

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{6}(U_k)^3 - \frac{1}{2}\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2}. \tag{66}$$

Second, we obtain discrete variational derivative of G_{d} according to (38) as

$$\frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} = \frac{1}{2}\frac{\left(U_k^{(n+1)}\right)^2 + U_k^{(n+1)}U_k^{(n)} + \left(U_k^{(n)}\right)^2}{3} + \delta_k^{\langle 2\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}. \tag{67}$$

Third, we obtain a scheme for the equation as

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 1\rangle}\left(\frac{1}{2}\frac{\left(U_k^{(n+1)}\right)^2 + U_k^{(n+1)}U_k^{(n)} + \left(U_k^{(n)}\right)^2}{3} + \delta_k^{\langle 2\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right). \tag{68}$$

This finite difference scheme is a new one for the KdV equation. Finally we obtain from (62) a discrete boundary condition as

$$U_{k+mN} = U_k, \qquad m \in \mathbf{Z}, \tag{69}$$

which satisfies (52), (53), and (56).

For $U_k^{(n)}$ computed through (68) and (69), the energy conservation property is inherited as

$$\sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(U^{(n)}\right)_k \Delta x = \sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(U^{(0)}\right)_k \Delta x \tag{70}$$

and the mass conservation property is inherited as

$$\sum_{k=0}^{N}{}'' U_k^{(n)} \Delta x = \sum_{k=0}^{N}{}'' U_k^{(0)} \Delta x. \tag{71}$$

We compute some numerical solutions for the KdV equation using our scheme (68). To solve the implicit scheme (68) numerically we use the Newton method. Figure 2 is one example of numerical solutions we obtained with $\Delta x = 1/20$ and $\Delta t = 1/10000$. With these parameters almost all schemes that are conditionally stable are unstable, for example, schemes in [17, 34]. Figure 3 shows the time dependency of energy of numerical solutions

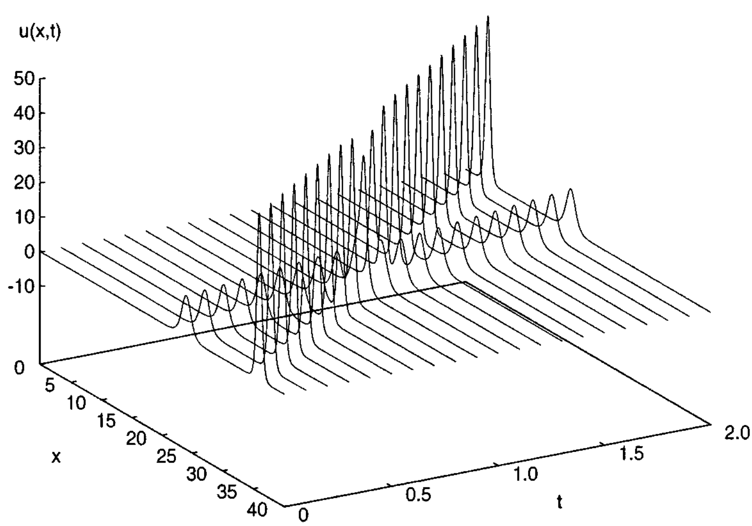

FIG. 2. Numerical solutions using our scheme (68) with $\Delta x = 1/20$, $\Delta t = 1/10000$, $\Omega = [0, 40]$. The initial value is $u(x, 0) = 48\ \mathrm{sech}^2(2(x - 36)) + 12\ \mathrm{sech}^2(x - 24)$, which is an approximation of the two-soliton solution.

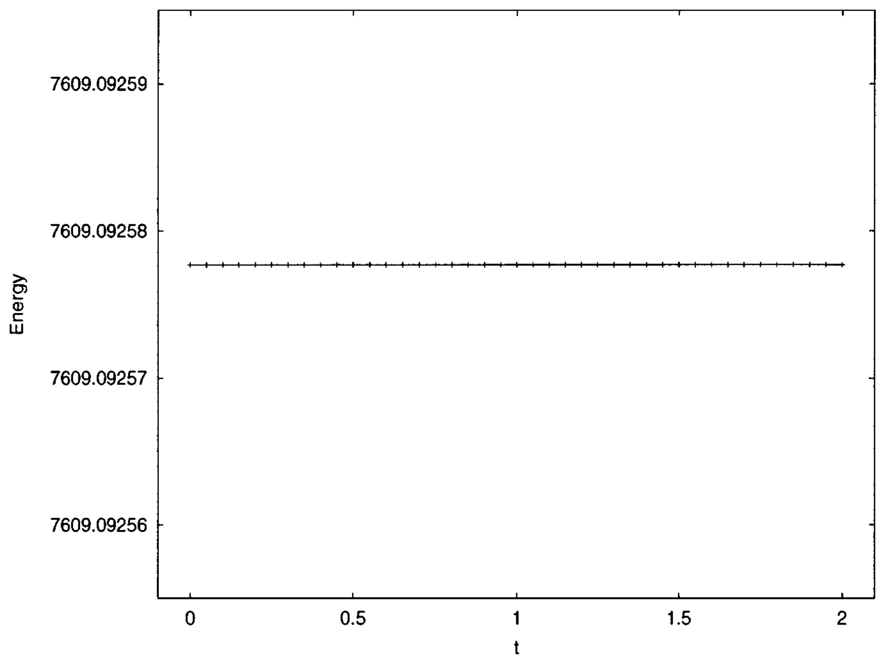

FIG. 3. The time dependency of energy of numerical solutions in Fig. 2. Theoretically, the energy conservation property is satisfied as (70).

in Fig. 2. As shown in the energy conservation property (70), the energy of numerical solutions ${\sum''}_{k=0}^{N} G_{\mathrm{d}}(U^{(n)})_k \Delta x$ is independent of time theoretically. Figure 3 indicates that the energy of numerical solutions is conserved quite well and agrees with the conservation property. Figure 4 shows the time dependency of mass of numerical solutions in Fig. 2. The mass of numerical solutions ${\sum''}_{k=0}^{N} U_k^{(n)} \Delta x$ is also independent of time theoretically and it is shown in the mass conservation property (71). In Fig. 4, the mass of numerical solutions are conserved quite well and it agrees with the conservation property also.

The latter two figures indicate that the conservation properties are also valid numerically, and Fig. 2 suggests that our scheme is also unconditionally stable. Note that our proposed method generates a new scheme and we expect that it has the above advantageous properties.

5.2. *Linear Diffusion Equation*

In this section we consider a linear diffusion equation as a simple example for $\alpha = 2$ in (2). This equation is a typical and well-known equation which needs stabilization, e.g., the Courant–Friedrichs–Lewy condition or the Crank–Nicolson scheme, to obtain numerical solutions. The equation is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{72}$$

and the boundary condition

$$[u u_x]_{x=0}^{L} = 0 \tag{73}$$

is imposed.

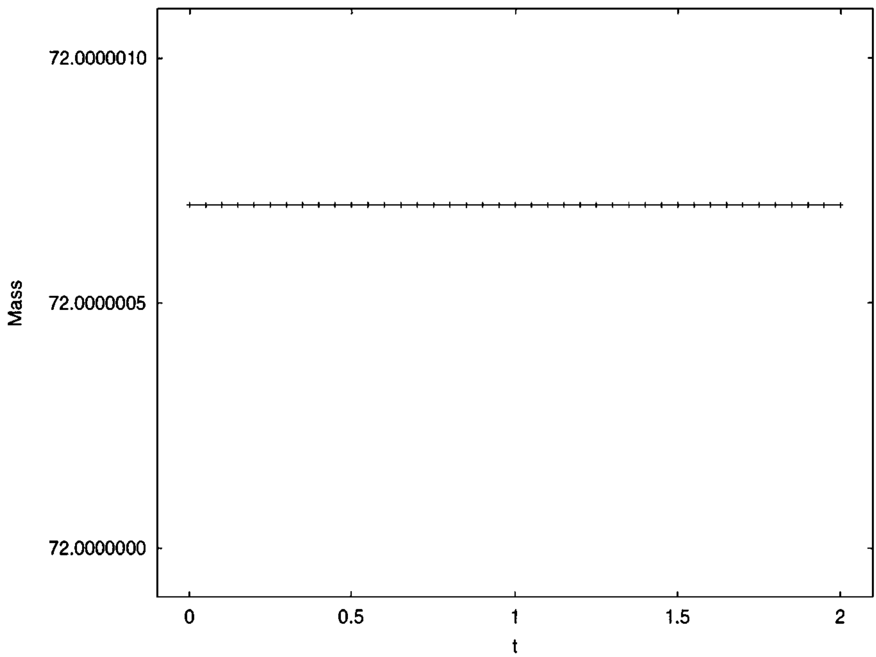

FIG. 4. The time dependency of mass of numerical solutions in Fig. 2. Theoretically, the mass conservation property is satisfied as (71).

This means that this equation is one instance of (2) with $\alpha = 2$ and

$$G(u, u_x) = \frac{1}{2}u^2, \tag{74}$$

and the condition (73) satisfies (4). From (74) we obtain $\partial G/\partial u_x = 0$ and this satisfies (3). For this system the total energy decreases, i.e.,

$$\frac{d}{dt}\int_0^L G(u, u_x)\, dx \le 0. \tag{75}$$

If $u(x, t)$ satisfies the optional condition (7), i.e.,

$$[u_x]_{x=0}^{L} = 0, \tag{76}$$

then the total mass is conserved, i.e.,

$$\frac{d}{dt}\int_0^L u(x, t)\, dx = 0. \tag{77}$$

According to Section 4, we obtain the scheme for this equation. First, we discretize "energy function" $G(u, u_x)$ of (74) to

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}(U_k)^2. \tag{78}$$

Second, we obtain the discrete variational derivative of G_{d} according to (38) as

$$\frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} = \frac{U_k^{(n+1)} + U_k^{(n)}}{2}. \tag{79}$$

Third, we obtain a scheme for the equation as

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right). \tag{80}$$

Finally we obtain discrete boundary conditions from (73) as

$$\left[\left(s_k^{\langle 1\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\left(\delta_k^{\langle 1\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right)\right]_{k=0}^{N} = 0, \tag{81}$$

which equals (53). For $U_k^{(n)}$, which satisfies (80) and (81), the energy dissipation property is inherited as

$$\sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}\left(U^{(n+1)}\right)_k \Delta x \le \sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}\left(U^{(n)}\right)_k \Delta x \qquad \text{for } n = 0, 1, 2, \ldots. \tag{82}$$

When the optional condition (76) is satisfied we discretize it as

$$\left[\delta_k^{\langle 1\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right]_{k=0}^{N} = 0, \tag{83}$$

which equals (56). We obtain the mass conservation property under this condition as

$$\sum_{k=0}^{N}{}'' \, U_k^{(n)}\Delta x = \sum_{k=0}^{N}{}'' \, U_k^{(0)}\Delta x. \tag{84}$$

Remark. The scheme (80) is identical with the Crank–Nicolson scheme [28, Section 8.2], which is unconditionally stable and is convergent with convergence rate $O((\Delta x)^2 + (\Delta t)^2)$.

5.3. *The Cahn–Hilliard Equation*

In this section we consider the Cahn–Hilliard equation [3] as an important example for $\alpha = 2$ in (2). This is a notorious equation for difficulty of numerical computation. In contrast to the abundant literature [6–8, 10] on FEM for the Cahn–Hilliard equation, there are relatively few studies on FDM [4, 16, 32]. Some numerical schemes are known to preserve some properties for the Cahn–Hilliard equation.

We show that we have to apply a quite small Δt for computing this equation if we use a conventional scheme [13]. With the scheme designed in this section, in contrast, we can obtain numerical solutions for the equation with an arbitrary Δt. The equation is

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right), \tag{85}$$

where $p < 0, q < 0$, and $0 < r$, and we suppose that the boundary conditions

$$\frac{\partial}{\partial x}u\bigg|_{x=0} = \frac{\partial}{\partial x}u\bigg|_{x=L} = 0, \tag{86}$$

$$\frac{\partial}{\partial x}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right)\bigg|_{x=0} = \frac{\partial}{\partial x}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right)\bigg|_{x=L} = 0, \tag{87}$$

i.e.,

$$\frac{\partial}{\partial x}u\bigg|_{x=0} = \frac{\partial}{\partial x}u\bigg|_{x=L} = 0, \tag{88}$$

$$\frac{\partial^3}{\partial x^3}u\bigg|_{x=0} = \frac{\partial^3}{\partial x^3}u\bigg|_{x=L} = 0, \tag{89}$$

are satisfied.

This equation is one instance of (2) with $\alpha = 2$ and

$$G(u, u_x) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q\left(\frac{\partial u}{\partial x}\right)^2, \tag{90}$$

and the condition (86) satisfies (3), while the condition (87) satisfies (4) and (7). For this system the total energy decreases, i.e.,

$$\frac{d}{dt}\int_0^L G(u, u_x)\,dx \leq 0, \tag{91}$$

and the total mass is conserved as

$$\frac{d}{dt}\int_0^L u(x, t)\,dx = 0. \tag{92}$$

According to Section 4, we obtain the scheme for this equation. First, we discretize “energy function” $G(u, u_x)$ of (90) to

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}p(U_k)^2 + \frac{1}{4}r(U_k)^4 - \frac{1}{2}q\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2}. \tag{93}$$

Second, we obtain the discrete variational derivative of G_{d} according to (38) as

$$\begin{aligned}\frac{\delta G_{\mathrm{d}}}{\delta\left(U^{(n+1)}, U^{(n)}\right)_k} = {} & p\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \\ & + r\frac{\left(U_k^{(n+1)}\right)^3 + \left(U_k^{(n+1)}\right)^2 U_k^{(n)} + U_k^{(n+1)}\left(U_k^{(n)}\right)^2 + \left(U_k^{(n)}\right)^3}{4} \\ & + q\delta_k^{\langle 2\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}.\end{aligned} \tag{94}$$

Third, we obtain a scheme for the equation

$$\begin{aligned}\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2\rangle} \Bigg\{ p\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \\ + r\frac{\big(U_k^{(n+1)}\big)^3 + \big(U_k^{(n+1)}\big)^2 U_k^{(n)} + U_k^{(n+1)}\big(U_k^{(n)}\big)^2 + \big(U_k^{(n)}\big)^3}{4} \\ + q\delta_k^{\langle 2\rangle}\, \frac{U_k^{(n+1)} + U_k^{(n)}}{2} \Bigg\}.\end{aligned} \tag{95}$$

Finally we obtain discrete boundary conditions from (88) and (89) as

$$\delta_k^{\langle 1\rangle} U_k^{(n)}\Big|_{k=0} = \delta_k^{\langle 1\rangle} U_k^{(n)}\Big|_{k=N} = 0 \tag{96}$$

$$\delta_k^{\langle 3\rangle} U_k^{(n)}\Big|_{k=0} = \delta_k^{\langle 3\rangle} U_k^{(n)}\Big|_{k=N} = 0. \tag{97}$$

These conditions satisfy (52), (53), and (56).

For $U_k^{(n)}$ computed through (94), (96), and (97), the energy dissipation property is inherited as

$$\sum_{k=0}^{N}{}'' \; G_{\mathrm{d}}\big(U^{(n+1)}\big)_k \Delta x \le \sum_{k=0}^{N}{}'' \; G_{\mathrm{d}}\big(U^{(n)}\big)_k \Delta x \tag{98}$$

and the mass conservation property as

$$\sum_{k=0}^{N}{}'' \; U_k^{(n)} \Delta x = \sum_{k=0}^{N}{}'' \; U_k^{(0)} \Delta x. \tag{99}$$

It is proved in [16] that the scheme (94) has the following properties:

- there is a unique solution $U_k^{(n+1)}$ for given $U_k^{(n)}$;
- the scheme is unconditionally stable;
- the scheme is convergent where the convergence rate is $O((\Delta x)^2 + (\Delta t)^2)$.

We computed some numerical solution for the Cahn–Hilliard equation using our scheme (94). To solve the implicit scheme (94) numerically we use the Newton method. Figure 5 is one example of numerical solutions we obtained. Figure 6 shows the time dependency of energy of numerical solutions in Fig. 5. As shown in the energy dissipation property (98), the energy of numerical solutions $\sum_{k=0}^{\prime\prime N} G_{\mathrm{d}}(U^{(n)})_k \Delta x$ theoretically decreases as time passes. Figure 6 indicates that the energy of numerical solutions decreases and agrees with the dissipation property. Figure 7 shows the time dependency of mass of numerical solutions in Fig. 5. The mass of numerical solutions $\sum_{k=0}^{\prime\prime N} U_k^{(n)} \Delta x$ is theoretically independent of time and this is shown in the mass conservation property (99). Looking at Fig. 7, the mass of numerical solutions is conserved quite well and it agrees with the conservation property also.

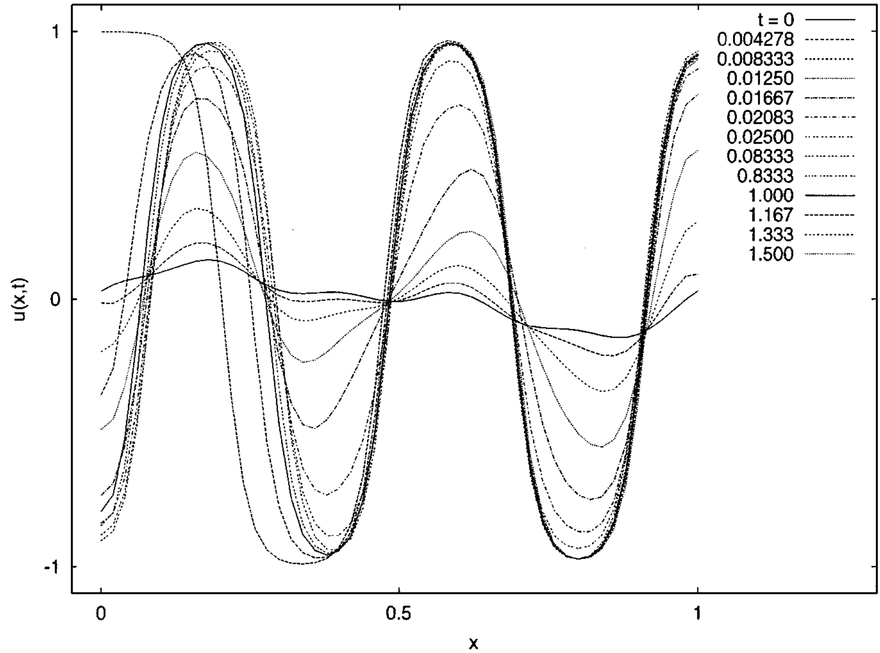

FIG. 5. Numerical solutions using our scheme (94) with $\Delta x = 1/50$, $\Delta t = 1/1200$, $\Omega = [0, 1]$, $p = -1.0$, $q = -0.001$, and $r = 1.0$. The initial value is $u(x, 0) = 0.1\sin(2\pi x) + 0.01\cos(4\pi x) + 0.06\sin(4\pi x) + 0.02\cos(10\pi x)$.

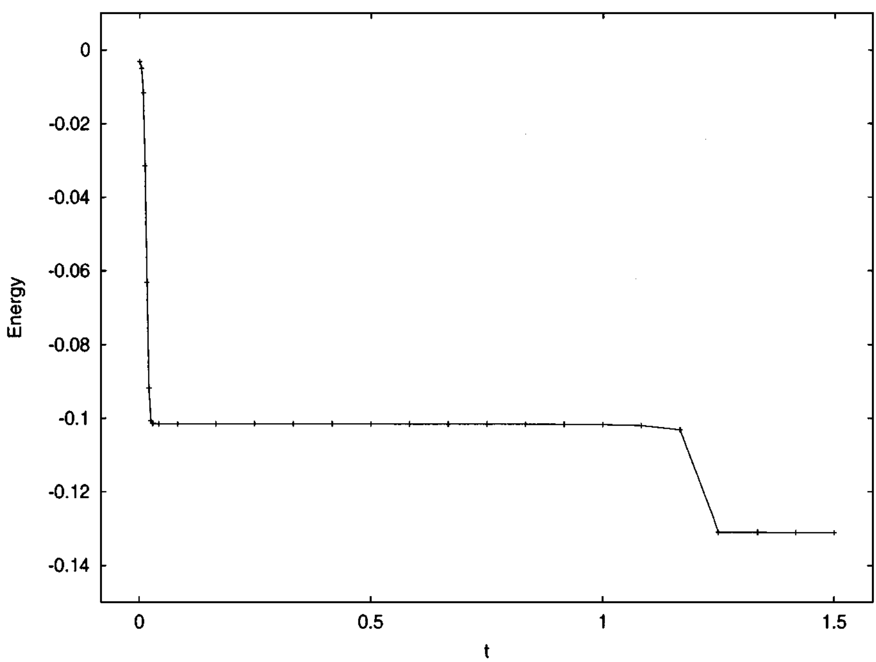

FIG. 6. The time dependency of energy of numerical solutions in Fig. 5. Theoretically, the energy dissipation property is satisfied as (98).

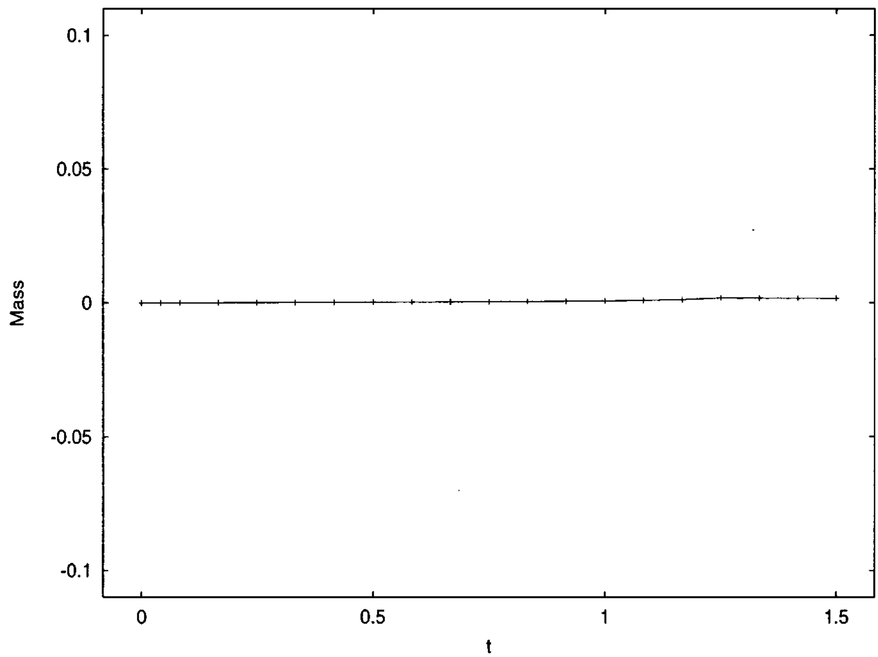

FIG. 7. The time dependency of mass of numerical solutions in Fig. 5. Theoretically, the mass conservation property is satisfied as (99).

The latter two figures indicate that the conservation properties are also valid numerically, and Fig. 5 suggests that our scheme is also unconditionally stable. These results agree with the dissipation/conservation properties and the stability proved in [16].

6. CONCLUSION

We have described a method for designing by rote finite difference schemes that inherit properties (5) (and (8)) from PDEs in (2). The proposed method is easy, simple, and applicable to many equations. The inherited properties are kept even if the time mesh size changes in the time-evolution process for the derived schemes. Some example schemes are derived through the proposed procedure and are shown to be superior to (competitive with) existing schemes in that they are consistent, stable, convergent, and flexible. This means that we may strongly expect that we can generate superior schemes for other PDEs easily.

Since all discrete basic operators we use are symmetric with respect to time reversal, the derived schemes must be implicit. This is by no means a drawback of the derived scheme. Computation time is sufficiently small using the derived schemes with relatively large Δt and we can take Δt large because the derived scheme is expected to be numerically stable. In addition to this, we can use appropriate time mesh adaptive methods for the derived schemes.

When the space dimension is more than one, discrete calculus is much more difficult and complicated except when space axes are orthogonal to each other. A simple discrete calculus when the space dimension is two is exemplified in [16].

APPENDIX: PROOF OF ITERATION OF SUMMATION BY PARTS

In this section we prove (35). For a matrix (or vector) A in general its transpose is denoted by A^{T}.

LEMMA A.1

$$\delta_k^{\langle h\rangle} = e^{\mathsf{T}} D_k^h e, \tag{A.1}$$

where

$$D_k \overset{\text{def}}{=} \begin{pmatrix} 0 & \delta_k^+ \\ \delta_k^- & 0 \end{pmatrix}, \tag{A.2}$$

$$e \overset{\text{def}}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{A.3}$$

Proof. This relation is trivial. ■

LEMMA A.2.

$$\sum_{k=0}^{N}{}'' \left\{ a_k D_k a_k' + \left(D_k a_k^{\mathsf{T}}\right)^{\mathsf{T}} a_k' \right\} \Delta x = \frac{1}{2}\left[a_k A_k a_k' + \left(A_k a_k^{\mathsf{T}}\right)^{\mathsf{T}} a_k' \right]_{k=0}^{N}, \tag{A.4}$$

where

$$a_k \overset{\text{def}}{=} \begin{pmatrix} \zeta_k & \eta_k \\ \theta_k & \xi_k \end{pmatrix}, \tag{A.5}$$

$$a_k' \overset{\text{def}}{=} \begin{pmatrix} \zeta_k' & \eta_k' \\ \theta_k' & \xi_k' \end{pmatrix}, \tag{A.6}$$

$$A_k \overset{\text{def}}{=} \begin{pmatrix} 0 & s_k^+ \\ s_k^- & 0 \end{pmatrix}. \tag{A.7}$$

Proof. From (34) we obtain this equation. ■

LEMMA A.3.

$$\begin{aligned} \sum_{k=0}^{N}{}'' \left\{ a_k D_k^h a_k' \right\} \Delta x &= (-1)^{h'} \sum_{k=0}^{N}{}'' \left(D_k^{h'} a_k^{\mathsf{T}}\right)^{\mathsf{T}} \left(D_k^{h-h'} a_k'\right) \Delta x \\ &\quad + \frac{1}{2}\left[\sum_{l=1}^{h'} (-1)^{l-1} \left\{ \left(D_k^{l-1} a_k^{\mathsf{T}}\right)^{\mathsf{T}} \left(A_k D_k^{h-l} a_k'\right) \right.\right. \\ &\quad \left.\left. + \left(A_k D_k^{l-1} a_k^{\mathsf{T}}\right)^{\mathsf{T}} \left(D_k^{h-l} a_k'\right) \right\} \right]_{k=0}^{N}, \end{aligned} \tag{A.8}$$

where $D_k^0 \overset{\text{def}}{=} I$, $h \in \mathbf{N}^+$, $h' \in \mathbf{N}$, *and* $h' \leq h$.

Proof. We obtain this equation from an iterative application of (A.4) to the LHS of this equation. ■

From this lemma and Lemma A.1 we obtain

$$\begin{aligned}\sum_{k=0}^{N}{}'' f_k \delta_k^{\langle h \rangle} f_k \Delta x = (-1)^{h'} \sum_{k=0}^{N}{}'' \left\{ e^{\top} \left(D_k^{h'} f_k \right)^{\top} \left(D_k^{h-h'} f_k \right) e \right\} \Delta x \\ + \frac{1}{2} \Bigg[\sum_{l=1}^{h'} (-1)^{l-1} \left\{ e^{\top} \left(D_k^{l-1} f_k \right)^{\top} \left(A_k D_k^{h-l} f_k \right) e \right\} \\ + \sum_{l=1}^{h'} (-1)^{l-1} \left\{ e^{\top} \left(A_k D_k^{l-1} f_k \right)^{\top} \left(D_k^{h-l} f_k \right) e \right\} \Bigg]_{k=0}^{N}, \end{aligned} \qquad \text{(A.9)}$$

where $h \in \mathbf{N}^{+}$, $h' \in \mathbf{N}$, and $h' \leq h$.

Substituting $h' = h/2$ into this equation we obtain (35) for even h. When h is odd, we obtain (35) by comparing this equation with $h' = (h-1)/2$ and $h' = (h+1)/2$.

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REFERENCES

1. W. F. Ames, *Nonlinear Partial Differential Equations in Engineering, I* (Academic Press, New York/London, 1965).
2. C. J. Budd and A. Iserles, Geometric integration: Numerical solution of differential equations on manifolds, in *Numerical Solution of Differential Equations on Manifolds*, edited by C. J. Budd and A. Iserles, *Philos. Trans. Roy. Soc. London Ser. A* **357**, 945 (1999).
3. J. W. Cahn and J. E. Hilliard, Free energy of a non-uniform system. I. Interfacial free energy, *J. Chem. Phys.* **28**, 258 (1958).
4. S. M. Choo and S. K. Chung, Conservative nonlinear difference scheme for the Cahn–Hilliard equation, *Comput. Math. Appl.* **36**, 31 (1998).
5. R. Courant, K. O. Friedrichs, and H. Lewy, Über die partiellen differenzengleichungen der mathematischen physik, *Math. Ann.* **100**, 32 (1928).
6. Q. Du and R. A. Nicolaides, Numerical analysis of a continuum model of phase transition, *SIAM J. Numer. Anal.* **28**, 1310 (1991).
7. C. M. Elliott and D. A. French, Numerical studies of the Cahn–Hilliard equation for phase separation, *IMA J. Appl. Math.* **38**, 97 (1987).
8. C. M. Elliott, D. A. French, and F. A. Milner, A second order splitting method for the Cahn–Hilliard equation, *Numer. Math.* **54**, 575 (1989).
9. T. Flå, A numerical energy conserving method for the DNLS equation, *J. Comput. Phys.* **101**, 71 (1992).
10. D. A. French and J. W. Schaeffer, Continuous finite element methods which preserve energy properties for nonlinear problems, *Appl. Math. Comput.* **39**, 271 (1990).
11. D. A. French and S. Jensen, Long-time behaviour of arbitrary order continuous time Galerkin schemes for some one-dimensional phase transition problems, *IMA J. Numer. Anal.* **14**, 421 (1994).
12. J. de Frutos and J. M. Sanz-Serna, Accuracy and conservation properties in numerical integration: The case of the Korteweg–de Vries equation, *Numer. Math.* **75**, 421 (1997).

13. D. Furihata, T. Onda, and M. Mori, A numerical analysis of equation by the finite difference scheme, *Trans. Jpn. Soc. Indust. Appl. Math.* **3**, 217 (1993). [in Japanese]

14. D. Furihata and M. Mori, Stability and convergence of difference schemes for the Cahn–Hilliard equation, in *Proceedings, Theory and Applications of Numerical Calculation in Science and Technology, Kyoto, Japan, 1995*, edited by T. Mitsui, Kokyuroku (RIMS, Kyoto Univ. 1996), No. 944, p. 235. [in Japanese]

15. D. Furihata and M. Mori, General derivation of finite difference schemes by means of a discrete variation, *Trans. Jpn. Soc. Indust. Appl. Math.* **8**, 317 (1998).

16. D. Furihata, An unconditionally stable finite difference scheme for the Cahn–Hilliard equation, submitted for publication.

17. I. S. Greig and J. Li. Morris, A Hopscotch method for the Korteweg–de-Vries equation, *J. Comput. Phys.* **20**, 64 (1976).

18. K. Goda, On instability of some finite difference schemes for the Korteweg–de Vries equation, *J. Phys. Soc. Jpn.* **39**, 229 (1975).

19. D. Greenspan, Conservative numerical methods for $\ddot{x} = f(x)$, *J. Comput. Phys.* **56**, 28 (1984).

20. R. L. Herman and C. J. Knickerbocker, Numerically induced phase shift in the KdV soliton, *J. Comput. Phys.* **104**, 50 (1993).

21. R. Hirota, Difference analogues of nonlinear evolution equations in Hamiltonian form, Hiroshima Univ. Tech. Rep., A-12, 1982.

22. J. M. Hyman and M. Shashkov, Mimetic discretizations for Maxwell's equations, *J. Comput. Phys.* **151**, 881 (1999).

23. P. W. Li, On the numerical study of the KdV equation by the semi-implicit and leap-frog method, *Comput. Phys. Comm.* **88**, 121 (1995).

24. S. Li and Vu-Quoc, Finite difference calculus invariant structure of a class of algorithms for the nonlinear Klein–Gordon equation, *SIAM J. Numer. Anal.* **32**, 1839 (1995).

25. R. I. McLachlan, G. R. W. Quispel, and G. S. Turner, Numerical integrators that preserve symmetries and reversing symmetries, *SIAM J. Numer. Anal.* **35**, 586 (1998).

26. R. A. Nicolaides, Direct discretization of planar div-curl problems, *SIAM J. Numer. Anal.* **29**, 32 (1992).

27. K. Pen-Yu and J. M. Sanz-Serna, Convergence of methods for the numerical solution of the Korteweg-de Vries equation, *IMA J. Numer. Anal.* **1**, 215 (1981).

28. R. D. Richtmyer and K. W. Morton, *Difference Methods for Initial-Value Problems* (Wiley, New York, 1967).

29. J. M. Sanz-Serna, An explicit finite-difference scheme with exact conservation properties, *J. Comput. Phys.* **47**, 199 (1982).

30. J. M. Sanz-Serna, Symplectic integrators for Hamiltonian problems: An overview, *Acta Numer.* **1**, 243 (1992).

31. W. Strauss and L. Vazquez, Numerical solution of a nonlinear Klein–Gordon equation, *J. Comput. Phys.* **28**, 271 (1978).

32. Z. Z. Sun, A second-order accurate linearized difference scheme for the two-dimensional Cahn–Hilliard equation, *Math. Comput.* **64**, 1463 (1995).

33. T. R. Taha and M. J. Ablowitz, Analytical and numerical aspects of certain nonlinear evolution equations. III. Numerical, Korteveg–de Vries equation, *J. Comput. Phys.* **55**, 231 (1984).

34. N. J. Zabusky and M. D. Kruskal, Interaction of "solitons" in a collisionless plasma and the recurrence of initial states, *Phys. Rev. Lett.* **15**, 240 (1965).