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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*

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Abstract

We propose a new procedure to design finite difference schemes that inherit the energy conservation or dissipation property from nonlinear partial differential equations, such as the Korteweg-de Vries equation and the Cahn-Hilliard equation. The most important feature of our procedure is a rigorous discretization of variational derivatives using summation by parts.

The inherited properties are satisfied exactly. Because of this we can expect that derived schemes are numerically stable and yield solutions converging to PDE solutions. We proved the stability and convergence of the scheme for the Cahn-Hilliard equation, and numerically verified the inheritance of the energy conservation and dissipation properties for KdV eq. and Cahn-Hilliard eq.

Key words. finite difference method, energy conservation, energy dissipation, KdV equation, Cahn-Hilliard equation

AMS subject classification. 65M06

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1 Introduction

We propose a procedure to design finite difference schemes that inherit the energy conservation or dissipation property from nonlinear partial differential equations.

The study of designing finite difference schemes that inherit a conservation property was begun by Courant, Friedrichs, and Lewy in 1928 [3]. This so-called "energy method" was primary studied to prove stability, existence and uniqueness of solutions of schemes in 1950's(Richtmyer and Morton [15, §6] well documented the results).

Since 1970's many studies are based on this method, for example, Strauss and Vazuquiez [17], Greenspan [10], Li and Vu-Quoc [13], and Fla [5]. For energy conservation, Strauss and Vazuquiez [17] discussed schemes for the linear Klein-Gordon equation and Greenspan [10] for initial value problem $\ddot{x} = f(x)$ and Li and Vu-Quoc [13] for the nonlinear Klein-Gordon equation. Fla [5] showed schemes that inherit energy conservation property and mass conservation property from DNLS equation. The famous "symplectic method" [16] that is applicable to Hamilton systems may be regarded as one application based on this formulation.

However, the main interest in the studies since 1970's shifts from stability to development of algorithms to compose schemes that inherit some characteristic properties of original equations. Li and Vu-Quoc [13] wrote the history well and said "*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*". As mentioned above many studies are done based on this formulation and make remarkable results.

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 [2] we must treat the dissipation laws as the property to inherit, too.

Through considering this problem we succeed in proposing a new finite difference scheme that inherits the energy dissipation property from the Cahn-Hilliard equation in [8]. Du and Nicolaides [4] also proposed an interesting FEM and an interesting FDM scheme that inherit the energy dissipation property for the equation under the Dirichlet boundary conditions. These results also exploit the possibility of unification of the conservation laws and the dissipation laws as the characteristic property to inherit.

In this paper we show a unified formulation to design finite difference schemes that inherit the conservation property or the dissipation property. The basis idea of this formulation has been reported in [7] without precise mathematical discussion.

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 $u_x = \dfrac{\partial u}{\partial x}$, and $\dfrac{\delta G}{\delta u}$ is a variational derivative of function $G(u, u_x)$ for u. Boundary conditions, properties of this family, definition of G, etc. are described in §2. The property of the equations for odd α to be inherited by the schemes is $\dfrac{\partial}{\partial t}\displaystyle\int G dx = 0$ and is called "energy conservation property" in this paper. When α is even it is $(-1)^{\frac{\alpha}{2}+1}\dfrac{\partial}{\partial t}\displaystyle\int G dx \leq 0$ and called "energy dissipation property". Under certain conditions "mass conservation property", $\dfrac{\partial}{\partial t}\displaystyle\int u(x,t)dx = 0$, is inherited in addition.

Now, the issue is if we can design the finite difference scheme that inherits the above properties for the equation (1). Our solution for this issue is to make discrete replicas of the cause-and-effect relationship between the equation (1) and the above properties in the context of exact finite difference calculus such like the summation–by–parts which corresponds to the integral–by–parts. In this paper we show that our attempt succeeds in solving the problem.

The contents of this paper are as follows. In §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 §3 definitions and properties of discrete operators are shown. In §4 we show the schemes designed to inherit the above properties. In §4.2 and §4.3 we prove that derived schemes inherit 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 §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. In §6 we summarize 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 the equation and its properties, which is described in this section, is fundamental for 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 "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 $\frac{\delta G}{\delta u} = \frac{\partial G}{\partial u} - \frac{d}{dx}\left(\frac{\partial G}{\partial u_x}\right)$.

We consider a class of boundary conditions which 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

$$\begin{cases} \left[\sum_{l=1}^{\frac{\alpha}{2}}(-1)^{l-1}F^{(l-1)}F^{(\alpha-1)}\right]_{x=0}^{L} = 0 & : \alpha \text{ is even} \\ \left[\sum_{l=1}^{\frac{\alpha-1}{2}}(-1)^{l-1}F^{(l-1)}F^{(\alpha-l)} + \frac{1}{2}(-1)^{\frac{\alpha-1}{2}}F^{(\frac{\alpha-1}{2})}F^{(\frac{\alpha-1}{2})}\right]_{x=0}^{L} = 0 & : \alpha \text{ is odd} \end{cases} \tag{4}$$

where $F^{(l)} \stackrel{\text{def}}{=} \left(\frac{\partial}{\partial x}\right)^{l}\frac{\delta G}{\delta u}$ 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 which satisfy two assumptions (3) and (4), time dependency of the integral of the energy function is indicated as follows.

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

where

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

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

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

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

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

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

For example, 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, pages 7,8]

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

and the Cahn-Hilliard equation [2]

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

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 the equation (5) must be discretized consistently. We choose one consistent "set" of discrete operators carefully for this purpose and describe them in §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 $s^+, s^-, s^{\langle 1\rangle}, \ldots$,

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

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

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

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

We define the n-th difference operator $\delta^{\langle n\rangle}$, which is discretization of the n-th differential operator, as

$$\delta^{\langle 1\rangle} \stackrel{\text{def}}{=} \frac{s^+ - s^-}{2\Delta x}, \tag{18}$$

$$\delta^{\langle 2\rangle} \stackrel{\text{def}}{=} \frac{s^+ - 2 + s^-}{\Delta x^2}, \tag{19}$$

$$\delta^{\langle 2m+1\rangle} \stackrel{\text{def}}{=} \delta^{\langle 1\rangle}\delta^{\langle 2m\rangle}, \qquad m \geq 1, \tag{20}$$

$$\delta^{\langle 2m+2\rangle} \stackrel{\text{def}}{=} \delta^{\langle 2\rangle}\delta^{\langle 2m\rangle}, \qquad m \geq 1. \tag{21}$$

We adopt these difference operators for the following reasons:

- operators should be "symmetric" (= they should not vary when $\Delta x \to -\Delta x$),

- number of reference points of the n-th difference operator should be $n+1$ (this number is minimum to approximate the differential operator),
- discrepancy between difference operator and differential operator should be minimum under above conditions.

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

$$\mu^{\langle 0\rangle} \stackrel{\text{def}}{=} 1, \tag{22}$$

$$\mu^{+} \stackrel{\text{def}}{=} \frac{1+s^{+}}{2}, \tag{23}$$

$$\mu^{-} \stackrel{\text{def}}{=} \frac{1+s^{-}}{2}, \tag{24}$$

$$\mu^{\langle 1\rangle} \stackrel{\text{def}}{=} \frac{\mu^{+}+\mu^{-}}{2} = \frac{1+s^{\langle 1\rangle}}{2}. \tag{25}$$

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

$$\sum_{k=0}^{N}{}'' f_k \Delta x \stackrel{\text{def}}{=} \left(\frac{1}{2} f_0 + \sum_{k=1}^{N-1} f_k + \frac{1}{2} f_N\right) \Delta x \tag{26}$$

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 $h > 0, h \in \mathbf{N}$.

$$\sum_{k=0}^{N}{}'' \delta^{\langle h\rangle} f_k \Delta x = \left[\mu^{\langle \sigma(h)\rangle} \delta^{\langle h-1\rangle} f_k\right]_{k=0}^{N} \tag{27}$$

$$\delta^{\langle h\rangle} \sum_{l=0}^{k}{}'' f_l \Delta x = \mu^{\langle \sigma(h)\rangle} \delta^{\langle h-1\rangle} f_k \tag{28}$$

where

$$[f_k]_{k=0}^{N} \stackrel{\text{def}}{=} f_N - f_0, \tag{29}$$

$$\sigma(h) \stackrel{\text{def}}{=} h \bmod 2 = \begin{cases} 0 & : \; h \text{ is even} \\ 1 & : \; h \text{ is odd.} \end{cases} \tag{30}$$

The following relationship is “summation by parts” that corresponds to integration by parts.

$$\sum_{k=0}^{N}{}'' f_k \left(\delta^{+} g_k\right) \Delta x + \sum_{k=0}^{N}{}'' \left(\delta^{-} f_k\right) g_k \Delta x = \left[\frac{f_k \left(s^{+} g_k\right) + \left(s^{-} f_k\right) g_k}{2}\right]_{k=0}^{N} \tag{31}$$

Repeated application of the summation by parts yields the following equation.

$$
\begin{aligned}
(32)\quad & \sum_{k=0}^{N}{}'' f_k \delta^{\langle h\rangle} f_k \Delta x \\
= & \begin{cases}
(-1)^{\frac{h}{2}} \displaystyle\sum_{k=0}^{N}{}'' \hat{F}_k^{\langle \frac{h}{2},h,2\rangle}\Delta x \\
\quad + \Bigg[\displaystyle\sum_{\substack{1\le l\le h/2 \\ l:\ \text{even}}} (-1)\frac{2\hat{F}^{\langle l-1\rangle}\hat{F}^{\langle h-l\rangle} + (\delta^{+}\hat{F}^{\langle l-2\rangle})(s^{+}\hat{F}^{\langle h-l\rangle}) + (\delta^{-}\hat{F}^{\langle l-2\rangle})(s^{-}\hat{F}^{\langle h-l\rangle})}{4} \\
\qquad + \displaystyle\sum_{\substack{1\le l\le h/2 \\ l:\ \text{odd}}} \frac{2\hat{F}^{\langle l-1\rangle}\hat{F}^{\langle h-l\rangle} + (s^{+}\hat{F}^{\langle l-2\rangle})(\delta^{+}\hat{F}^{\langle h-l\rangle}) + (s^{-}\hat{F}^{\langle l-2\rangle})(\delta^{-}\hat{F}^{\langle h-l\rangle})}{4} \Bigg]_{k=0}^{N} \\
\hfill : h \text{ is even} \\
\Bigg[\displaystyle\sum_{\substack{1\le l\le (h-1)/2 \\ l:\ \text{even}}} (-1)\frac{(\delta^{+}\hat{F}^{\langle l-2\rangle})(\delta^{+}\hat{F}^{\langle h-l-1\rangle}) + (\delta^{-}\hat{F}^{\langle l-2\rangle})(\delta^{-}\hat{F}^{\langle h-l-1\rangle})}{2} \\
\quad + \displaystyle\sum_{\substack{1\le l\le (h-1)/2 \\ l:\ \text{odd}}} \frac{\hat{F}^{\langle l-1\rangle}(s^{\langle 1\rangle}\hat{F}^{\langle h-l\rangle}) + (s^{\langle 1\rangle}\hat{F}^{\langle l-1\rangle})\hat{F}^{\langle h-l\rangle}}{2} \\
\qquad + \dfrac{1}{2}(-1)^{\frac{h-1}{2}}\hat{F}^{\langle \frac{h-1}{2},h,2\rangle} \Bigg]_{k=0}^{N}, \\
\hfill : h \text{ is odd}
\end{cases}
\end{aligned}
$$

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

$$
(33)\qquad \hat{F}_k^{\langle l\rangle} \stackrel{\text{def}}{=} \delta^{\langle l\rangle} f_k,
$$

$$
(34)\qquad \hat{F}^{\langle l,l',2\rangle} \stackrel{\text{def}}{=} \begin{cases} \hat{F}^{\langle l\rangle}\left(s^{\langle \sigma(l')\rangle}\hat{F}^{\langle l\rangle}\right) & : \ l \text{ is even} \\ \dfrac{(\delta^{+}\hat{F}^{\langle l-1\rangle})^2 + (\delta^{-}\hat{F}^{\langle l-1\rangle})^2}{2} & : \ l \text{ is odd} \end{cases}
$$

for $l, l' \in \mathbf{N}$. The derivation of (32) is shown in Appendix.

3.3 Discrete Variational Derivative

In this subsection we describe definition and properties of the discrete variational derivative which is derived from the definitions in §3.1 using relations in §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 following form:

$$G_{\mathrm{d}}(U)_k \quad = \quad \sum_{l=1}^{m} f_l(U_k)\ g_l^+(\delta^+ U_k)\ g_l^-(\delta^- U_k), \qquad k \in \mathbf{Z} \tag{35}$$

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

$$\begin{aligned} \left(\frac{\delta G_{\mathrm{d}}}{\delta(U,V)} \right)_k \quad \stackrel{\text{def}}{=} \quad \sum_{l=1}^{m} \Bigg(& \frac{df_l}{d(U_k,V_k)} \frac{g_l^+(\delta^+ U_k) g_l^-(\delta^- U_k) + g_l^+(\delta^+ V_k) g_l^-(\delta^- V_k)}{2} \\ & - \delta^+ W_l^-(U,V)_k - \delta^- W_l^+(U,V)_k \Bigg) \end{aligned} \tag{36}$$

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

$$W_l^+(U,V)_k = \left(\frac{f_l(U_k) + f_l(V_k)}{2} \right) \left(\frac{g_l^-(\delta^- U_k) + g_l^-(\delta^- V_k)}{2} \right) \frac{dg_l^+}{d(\delta^+ U_k, \delta^+ V_k)} \tag{37}$$

$$W_l^-(U,V)_k = \left(\frac{f_l(U_k) + f_l(V_k)}{2} \right) \left(\frac{g_l^+(\delta^+ U_k) + g_l^+(\delta^+ V_k)}{2} \right) \frac{dg_l^-}{d(\delta^- U_k, \delta^- V_k)} \tag{38}$$

$$\frac{df}{d(a,b)} \stackrel{\text{def}}{=} \begin{cases} \dfrac{f(a) - f(b)}{a - b} & : \ a \neq b \\ \dfrac{df}{da} & : \ a = b. \end{cases} \tag{39}$$

We note that this definition is well-defined.

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

$$J[u] - J[v] \cong \int_\Omega \frac{\delta G}{\delta u}(u - v)dx + \left[\frac{\partial G}{\partial u_x}(u - v) \right]_{\partial\Omega} \tag{40}$$

where

$$J[u] \stackrel{\text{def}}{=} \int_\Omega G(u)dx. \tag{41}$$

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

$$J_{\mathrm{d}}[U] = \sum_{k=0}^{N}{}'' \ G_{\mathrm{d}}(U)_k \Delta x. \tag{42}$$

By the summation by parts (31) applied to difference $J_{\mathrm{d}}[U] - J_{\mathrm{d}}[V]$ we obtain

(43) $J_{\mathrm{d}}[U] - J_{\mathrm{d}}[V]$

$$= \sum_{k=0}^{N}{}'' \left\{ \sum_{l=1}^{m} \left(\frac{df_l}{d(U_k, V_k)} \frac{g_l^+(\delta^+ U_k) g_l^-(\delta^- U_k) + g_l^+(\delta^+ V_k) g_l^-(\delta^- V_k)}{2} \right.\right.$$

$$\left.\left. - \delta^+ W_l^-(U,V)_k - \delta^- W_l^+(U,V)_k \right) \right\} (U_k - V_k)\Delta x$$

$$+ \left[\frac{1}{2} \sum_{l=1}^{m} \left(W_l^+(U,V)_k \; s^+(U_k - V_k) + W_l^-(U,V)_k \; s^-(U_k - V_k) \right.\right.$$

$$\left.\left. + \left(s^+ W_l^-(U,V)_k + s^- W_l^+(U,V)_k \right) (U_k - V_k) \right) \right]_{k=0}^{N}$$

$$= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(U,V)}_k (U_k - V_k)\Delta x + \left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U,V)_k \right]_{k=0}^{N},$$

where

(44) $$\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U,V)_k \stackrel{\mathrm{def}}{=}$$
$$\frac{1}{2} \sum_{l=1}^{m} \left(W_l^+(U,V)_k \; s^+(U_k - V_k) + W_l^-(U,V)_k \; s^-(U_k - V_k) \right.$$
$$\left. + \left(s^+ W_l^-(U,V)_k + s^- W_l^+(U,V)_k \right) (U_k - V_k) \right).$$

This yields the following equation :

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

if $\left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U,V)_k \right]_{k=0}^{N} = 0$. The equation (43) may be regarded as a discrete analogue of (40).
Remark : In more general case where G involves u_{xx}, u_{xxx}, etc., the discrete variational derivative of G can be treated in a similar manner, which 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.

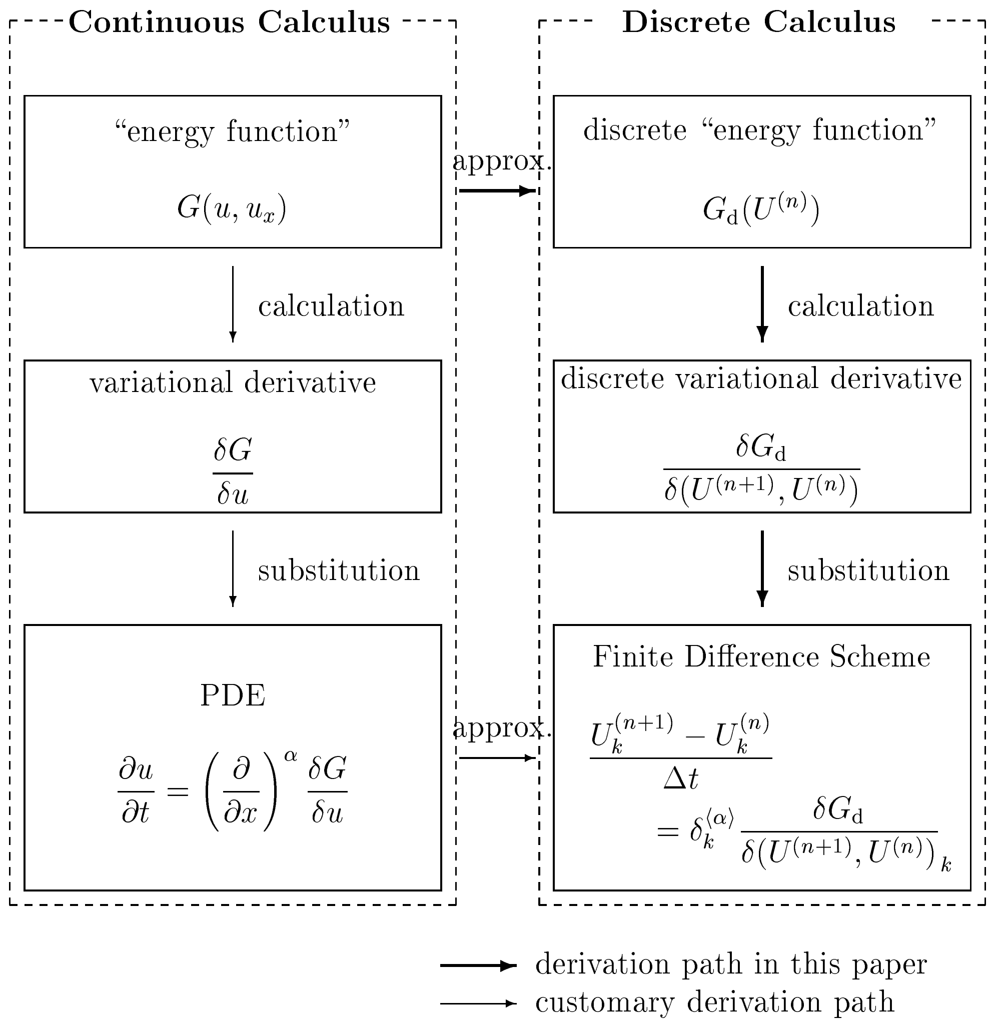

Figure 1: Design flow chart of the finite difference scheme

Recall our assumption on the discretization of the energy function G that G_{d} must be in the form (35). This is because we use the discrete variational derivative of G_{d}.

4.1 The Finite Difference Method

For the equation $\dfrac{\partial u}{\partial t} = \left(\dfrac{\partial}{\partial x}\right)^{\alpha} \dfrac{\delta G}{\delta u}$ in (2) with $\alpha \in \mathbf{N}$, we propose the following finite difference scheme

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta^{\langle \alpha \rangle} \frac{\delta G_{\mathrm{d}}}{\delta (U^{(n+1)}, U^{(n)})}_k, \qquad 0 \le k \le N, k \in \mathbf{Z}, n \in \mathbf{N} \tag{46}$$

with discrete boundary conditions. We note that the proposed scheme (46) involves $\left(U_k^{(n+1)}\right)_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ and $\left(U_k^{(n)}\right)_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ where
$(a_k)_{k=m_1}^{m_2} \stackrel{\mathrm{def}}{=} \{a_{m_1}, a_{m_1+1}, a_{m_1+2}, \ldots, a_{m_2}\}$,

$$\alpha'' \stackrel{\mathrm{def}}{=} \left\lceil \frac{\alpha}{2} \right\rceil \tag{47}$$

and

$$\beta = \beta(G_{\mathrm{d}}) \stackrel{\mathrm{def}}{=} \begin{cases} 0 & : \ g_l^+ = \text{const. and } g_l^- = \text{const. for } 1 \le {}^{\forall} l \le m \\ 1 & : \ \text{not in above case and} \\ & \quad\ g_l^+ = \text{const. or } g_l^- = \text{const. for } 1 \le {}^{\forall} l \le m \\ 2 & : \ \text{otherwise} \end{cases} \tag{48}$$

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

The First Constraint:
$\left(U_k^{(n+1)}\right)_{k=-\alpha''-\beta}^{-1}$ and $\left(U_k^{(n+1)}\right)_{k=N+1}^{N+\alpha''+\beta}$ must be described explicitly with $\left(U_k^{(n)}\right)_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ and $\left(U_k^{(n+1)}\right)_{k=0}^{N}$ through the discrete boundary conditions. This also implies that $\left(U_k^{(0)}\right)_{k=-\alpha''-\beta}^{N+\alpha''+\beta}$ are given. This constraint is necessary for the well-posedness of the proposed scheme (46).

The Second Constraint:
This corresponds to the ones (3),(4) in the continuous context. The first one, which corresponds to (3), is

$$\left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U^{(n+1)}, U^{(n)})_k\right]_{k=0}^{N} = 0. \tag{49}$$

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

$$
\begin{cases}
\Bigg[\displaystyle\sum_{\substack{1\le l\le \alpha/2 \\ l:\ \mathrm{even}}} (-1) \frac{2\tilde{F}^{\langle l-1\rangle}\tilde{F}^{\langle \alpha-l\rangle} + (\delta^{+}\tilde{F}^{\langle l-2\rangle})(s^{+}\tilde{F}^{\langle \alpha-l\rangle}) + (\delta^{-}\tilde{F}^{\langle l-2\rangle})(s^{-}\tilde{F}^{\langle \alpha-l\rangle})}{4} \\
\quad + \displaystyle\sum_{\substack{1\le l\le \alpha/2 \\ l:\ \mathrm{odd}}} \frac{2\tilde{F}^{\langle l-1\rangle}\tilde{F}^{\langle \alpha-l\rangle} + (s^{+}\tilde{F}^{\langle l-2\rangle})(\delta^{+}\tilde{F}^{\langle \alpha-l\rangle}) + (s^{-}\tilde{F}^{\langle l-2\rangle})(\delta^{-}\tilde{F}^{\langle \alpha-l\rangle})}{4} \Bigg]_{k=0}^{N} \\
\qquad = 0 \\
\qquad : \alpha \text{ is even} \\
\Bigg[\displaystyle\sum_{\substack{1\le l\le (\alpha-1)/2 \\ l:\ \mathrm{even}}} (-1) \frac{(\delta^{+}\tilde{F}^{\langle l-2\rangle})(\delta^{+}\tilde{F}^{\langle \alpha-l-1\rangle}) + (\delta^{-}\tilde{F}^{\langle l-2\rangle})(\delta^{-}\tilde{F}^{\langle \alpha-l-1\rangle})}{2} \\
\quad + \displaystyle\sum_{\substack{1\le l\le (\alpha-1)/2 \\ l:\ \mathrm{odd}}} \frac{\tilde{F}^{\langle l-1\rangle}(s^{\langle 1\rangle}\tilde{F}^{\langle \alpha-l\rangle}) + (s^{\langle 1\rangle}\tilde{F}^{\langle l-1\rangle})\tilde{F}^{\langle \alpha-l\rangle}}{2} \\
\qquad + \frac{1}{2}(-1)^{\frac{\alpha-1}{2}}\tilde{F}^{\langle \frac{\alpha-1}{2},\alpha,2\rangle} \Bigg]_{k=0}^{N} = 0 \\
\qquad : \alpha \text{ is odd}
\end{cases}
\tag{50}
$$

where

$$
\tilde{F}^{\langle l\rangle} \stackrel{\mathrm{def}}{=} \delta^{\langle l\rangle}\frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)},U^{(n)})_k}, \tag{51}
$$

$$
\tilde{F}^{\langle l,l',2\rangle} \stackrel{\mathrm{def}}{=} \begin{cases} \tilde{F}^{\langle l\rangle}\left(s^{\langle\sigma(l')\rangle}\tilde{F}^{\langle l\rangle}\right) & : \quad l \text{ is even} \\ \dfrac{(\delta^{+}\tilde{F}^{\langle l-1\rangle})^2 + (\delta^{-}\tilde{F}^{\langle l-1\rangle})^2}{2} & : \quad l \text{ is odd.} \end{cases} \tag{52}
$$

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

$$
\begin{cases} \displaystyle\sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)},U^{(n)})_k}\Delta x & = & 0 & : & \alpha = 0 \\ \left[\mu^{\langle\sigma(\alpha)\rangle}\delta^{\langle\alpha-1\rangle}\dfrac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)},U^{(n)})_k}\right]_{k=0}^{N} & = & 0 & : & \alpha > 0. \end{cases} \tag{53}
$$

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 **1 (energy conservation)** *Let $U_k^{(n)}$ be computed through (46), (49) and (50) for odd α. Then the total energy $\sum_{k=0}^{N}{}'' \, G_d(U^{(n)})_k \Delta x$ is independent of time step n.*

Proof :

$$\begin{aligned}
(54) \qquad & \frac{1}{\Delta t}\left\{ \sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}(U^{(n+1)})_k \Delta x - \sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}(U^{(n)})_k \Delta x \right\} \\
&= \sum_{k=0}^{N}{}'' \, \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k} \left(\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} \right) \Delta x \\
&= \sum_{k=0}^{N}{}'' \, \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k} \cdot \delta^{\langle \alpha \rangle} \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k} \Delta x \\
&= \mathrm{LHS}(50) \\
&= 0.
\end{aligned}$$

The first equality is derived from (45) and (49). The second is from the scheme (46). The third is from (32). The last is from (50). □

THEOREM **2 (mass conservation)** *Let $U_k^{(n)}$ be computed through (46), (49) and (50) for odd α. If the optional condition (53) 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 :

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

The first equality is derived from the scheme (46). The second is from (27) The last is from the optional condition (53). □

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 **3 (energy dissipation)** *Let $U_k^{(n)}$ be computed through (46), (49) and (50) for even α. Then the (sign-modified) total energy $(-1)^{\frac{\alpha}{2}+1} \sum_{k=0}^{N}{}'' \, G_d(U^{(n)})_k \Delta x$ decreases as the time step n increases.*

Proof :

$$
\begin{aligned}
(56) \qquad & \frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}(U^{(n+1)})_k \Delta x - \sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}(U^{(n)})_k \Delta x\right\} \\
&= \sum_{k=0}^{N}{}'' \, \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})}_k \left(\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t}\right) \Delta x \\
&= \sum_{k=0}^{N}{}'' \, \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})}_k \cdot \delta^{\langle\alpha\rangle} \frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})}_k \Delta x \\
&= \mathrm{LHS}(50) + (-1)^{\alpha/2} \sum_{k=0}^{N}{}'' \, \tilde{F}^{\langle \frac{\alpha}{2}, \alpha, 2\rangle} \Delta x \\
&= (-1)^{\alpha/2} \cdot (\mathrm{NonNegative})
\end{aligned}
$$

where $\tilde{F}^{\langle l\rangle}$ is defined in (51). The first equality is derived from (45) and (49). The second is from the scheme (46). The third is from (32). The last is from (50). □

THEOREM **4 (mass conservation)** *Let $U_k^{(n)}$ be computed through (46), (49) and (50) for even α. If the optional condition (53) 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 :

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

$$
\begin{aligned}
&= \begin{cases} \displaystyle\sum_{k=0}^{N}{}'' \frac{\delta G_{\rm d}}{\delta(U^{(n+1)}, U^{(n)})}_k \Delta x & : \quad \alpha = 0 \\ \displaystyle\left[\delta^{\langle \alpha - 1 \rangle} \frac{\delta G_{\rm d}}{\delta(U^{(n+1)}, U^{(n)})}_k\right]_{k=0}^{N} & : \quad \alpha > 0 \end{cases} \\
&= \ 0.
\end{aligned}
$$

The first equality is derived from the scheme (46). The second is from (27) The last is from the optional condition (53). □

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 [9],[14], although Li [12] proposes an unconditionally stable scheme. The equation is

$$
\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{1}{2}u^2 + \frac{\partial^2 u}{\partial x^2}\right\} \tag{58}
$$

and the periodic condition

$$
u(x + nL) = u(x), \qquad n \in \mathbf{Z} \tag{59}
$$

is imposed.

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

$$
G(u, u_x) = \frac{1}{6}u^3 - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2, \tag{60}
$$

and the condition (59) satisfies (3) and (4). For this system the total energy is conserved, i.e.,

$$
\frac{d}{dt}\int_0^L G(u, u_x)dx = 0. \tag{61}
$$

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

$$
\frac{d}{dt}\int_0^L u(x,t)dx = 0. \tag{62}
$$

According to §4, we obtain the scheme for this equation. Firstly, we discretize "energy function" $G(u, u_x)$ of (60) to

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{6}(U_k)^6 - \frac{1}{2}\frac{(\delta^+ U_k)^2 + (\delta^- U_k)^2}{2}. \tag{63}$$

Secondly we obtain discrete variational derivative of G_{d} according to (36) as

$$\frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k} = \frac{1}{2}\frac{(U_k^{(n+1)})^2 + U_k^{(n+1)}U_k^{(n)} + (U_k^{(n)})^2}{3} + \delta^{\langle 2\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}. \tag{64}$$

Thirdly we obtain a scheme for the equation as

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta^{\langle 1\rangle}\left(\frac{1}{2}\frac{(U_k^{(n+1)})^2 + U_k^{(n+1)}U_k^{(n)} + (U_k^{(n)})^2}{3} + \delta^{\langle 2\rangle}\frac{U_k^{(n+1)} + U_k^{(n)}}{2}\right). \tag{65}$$

Finally we obtain from (59) a discrete boundary condition as

$$U_{k+mN} = U_k, \qquad m \in \mathbf{Z}, \tag{66}$$

which satisfies (49), (50) and (53).

For $U_k^{(n)}$ computed through (65) and (66), the energy conservation property is inherited as

$$\sum_{k=0}^{N}{}'' \; G_{\mathrm{d}}(U^{(n)})_k \Delta x = \sum_{k=0}^{N}{}'' \; G_{\mathrm{d}}(U^{(0)})_k \Delta x \tag{67}$$

and the mass conservation property is inherited as

$$\sum_{k=0}^{N}{}'' \; U_k^{(n)} \Delta x = \sum_{k=0}^{N}{}'' \; U_k^{(0)} \Delta x. \tag{68}$$

We computed some numerical solutions for the KdV eq. using our scheme (65). Figure 2 is one example of numerical solutions we obtained with $\Delta x = 1/20$ and $\Delta t = 1/1000$. With these parameters almost all schemes including the Hopscotch scheme in [9] are unstable while Li's stable scheme [12] works. Note that this means our scheme is also unconditionally stable.

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

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{69}$$

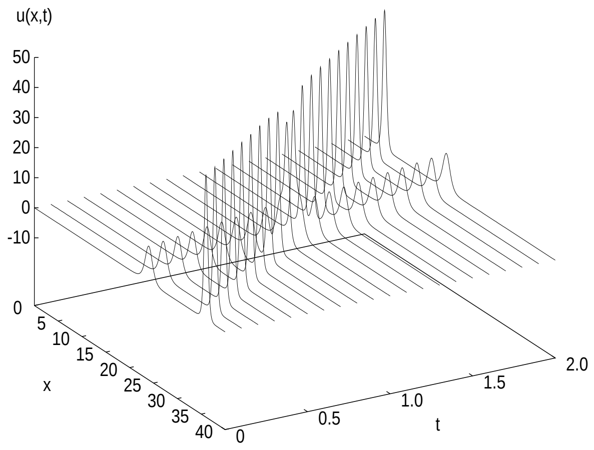

Figure 2: Numerical solutions using our scheme (65) with $\Delta x = 1/20$, $\Delta t = 1/1000$, $\Omega = [0, 40]$. The initial data is $u(x, 0) = 48 \operatorname{sech}^2(2(x - 36)) + 12 \operatorname{sech}^2(x - 24)$ which is an approximation of the two-soliton solution.

and the boundary condition

$$[uu_x]_{x=0}^{L} = 0 \tag{70}$$

is imposed.

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

$$G(u, u_x) = \frac{1}{2}u^2, \tag{71}$$

and the condition (70) satisfies (4). From (71) we obtain $\dfrac{\partial G}{\partial u_x} = 0$ and this satisfies (3). For this system the total energy decreases, i.e.,

$$\frac{d}{dt}\int_0^L G(u, u_x)dx \leq 0. \tag{72}$$

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

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

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

$$\frac{d}{dt}\int_0^L u(x, t)dx = 0. \tag{74}$$

According to §4, we obtain the scheme for this equation. Firstly, we discretize "energy function" $G(u, u_x)$ of (71) to

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}\left(U_k\right)^2. \tag{75}$$

Secondly we obtain the discrete variational derivative of G_{d} according to (36) as

$$\frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k} = \frac{U_k^{(n+1)} + U_k^{(n)}}{2}. \tag{76}$$

Thirdly we obtain a scheme for the equation as

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta^{\langle 2\rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right). \tag{77}$$

Finally we obtain discrete boundary conditions from (70) as

$$\left[\left(s^{\langle 1\rangle} \frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \left(\delta^{\langle 1\rangle} \frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) \right]_{k=0}^{N} = 0, \tag{78}$$

which equals to (50). For $U_k^{(n)}$ which satisfies (77) and (78), the energy dissipation property is inherited as

$$\sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}(U^{(n+1)})_k \Delta x \le \sum_{k=0}^{N}{}'' \, G_{\mathrm{d}}(U^{(n)})_k \Delta x \quad \text{for} \ \ n = 0, 1, 2, \ldots. \tag{79}$$

When the optional condition (73) is satisfied we discretize it as

$$\left[\delta^{\langle 1\rangle} \frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right]_{k=0}^{N} = 0, \tag{80}$$

which equals to (53). We obtain the mass conservation property under this condition as

$$\sum_{k=0}^{N}{}'' \, U_k^{(n)} \Delta x = \sum_{k=0}^{N}{}'' \, U_k^{(0)} \Delta x. \tag{81}$$

Remark : The scheme (77) is identical with the Crank-Nicolson scheme [15, §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 [2] as an important example for $\alpha = 2$ in (2). This is a notorious equation for difficulty of numerical computation [8], [18]. We show that we have to apply a quite small Δt for computing this equation if we use a conventional scheme [6]. With the scheme designed in this section, in contrast, we can obtain numerical solutions for the equation with an arbitrary Δt . The equation is

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right) \tag{82}$$

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

$$\left.\frac{\partial}{\partial x}u\right|_{x=0} = \left.\frac{\partial}{\partial x}u\right|_{x=L} = 0, \tag{83}$$

$$\left.\frac{\partial}{\partial x}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right)\right|_{x=0} = \left.\frac{\partial}{\partial x}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right)\right|_{x=L} = 0, \tag{84}$$

i.e.

$$\left.\frac{\partial}{\partial x}u\right|_{x=0} = \left.\frac{\partial}{\partial x}u\right|_{x=L} = 0, \tag{85}$$

$$\left.\frac{\partial^3}{\partial x^3}u\right|_{x=0} = \left.\frac{\partial^3}{\partial x^3}u\right|_{x=L} = 0 \tag{86}$$

are satisfied.

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

$$G(u, u_x) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(\frac{\partial u}{\partial x})^2, \tag{87}$$

and the condition (83) satisfies (3) and the condition (84) satisfies (4) and (7). For this system the total energy decreases, i.e.,

$$\frac{d}{dt}\int_0^L G(u, u_x)dx \le 0 \tag{88}$$

and the total mass is conserved as

$$\frac{d}{dt}\int_0^L u(x, t)dx = 0. \tag{89}$$

According to §4, we obtain the scheme for this equation. Firstly, we discretize "energy function" $G(u, u_x)$ of (87) to

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}p\left(U_k\right)^2 + \frac{1}{4}r\left(U_k\right)^4 - \frac{1}{2}q\frac{\left(\delta^+ U_k\right)^2 + \left(\delta^- U_k\right)^2}{2}. \tag{90}$$

Secondly we obtain the discrete variational derivative of G_{d} according to (36) as

$$\frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})_k} \tag{91}$$

$$
\begin{aligned}
= \ & p\frac{U_k^{(n+1)}+U_k^{(n)}}{2} \\
& +r\frac{(U_k^{(n+1)})^3+(U_k^{(n+1)})^2U_k^{(n)}+U_k^{(n+1)}(U_k^{(n)})^2+(U_k^{(n)})^3}{4} \\
& +q\ \delta^{\langle 2\rangle}\frac{U_k^{(n+1)}+U_k^{(n)}}{2}.
\end{aligned}
$$

Thirdly we obtain a scheme for the equation as

$$
\begin{aligned}
& \frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t} \\
& = \delta^{\langle 2\rangle}\left\{ p\frac{U_k^{(n+1)}+U_k^{(n)}}{2} \right. \\
& \quad +r\frac{(U_k^{(n+1)})^3+(U_k^{(n+1)})^2U_k^{(n)}+U_k^{(n+1)}(U_k^{(n)})^2+(U_k^{(n)})^3}{4} \\
& \quad \left. +q\ \delta^{\langle 2\rangle}\frac{U_k^{(n+1)}+U_k^{(n)}}{2} \right\}.
\end{aligned} \tag{92}
$$

Finally we obtain discrete boundary conditions from (85) and (86) as

$$
\delta^{\langle 1\rangle}U_k^{(n)}\Big|_{k=0} = \delta^{\langle 1\rangle}U_k^{(n)}\Big|_{k=N} = 0 \tag{93}
$$

$$
\delta^{\langle 3\rangle}U_k^{(n)}\Big|_{k=0} = \delta^{\langle 3\rangle}U_k^{(n)}\Big|_{k=N} = 0. \tag{94}
$$

These conditions satisfy (49), (50) and (53).

For $U_k^{(n)}$ computed through (92), (93) and (94), the energy dissipation property is inherited as

$$
\sum_{k=0}^{N}{}'' \ G_{\mathrm{d}}(U^{(n+1)})_k\Delta x \le \sum_{k=0}^{N}{}'' \ G_{\mathrm{d}}(U^{(n)})_k\Delta x \tag{95}
$$

and the mass conservation property as

$$
\sum_{k=0}^{N}{}'' \ U_k^{(n)}\Delta x = \sum_{k=0}^{N}{}'' \ U_k^{(0)}\Delta x. \tag{96}
$$

It is proved in [8] that the scheme (92) 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 solutions for the Cahn-Hilliard eq. using our scheme (92). Figure 3 is one example of numerical solutions we obtained.

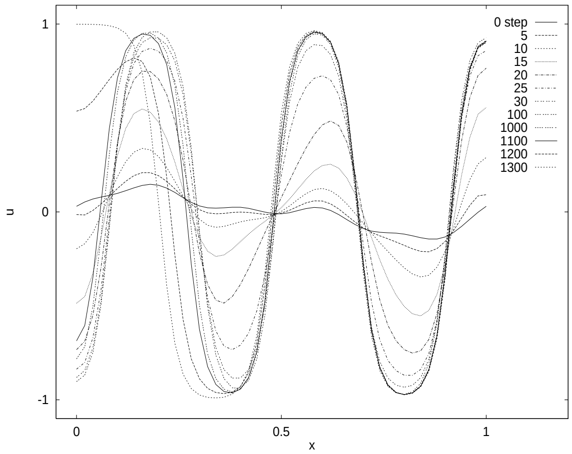

Figure 3: Numerical solutions using our scheme (92) with $\Delta x = 1/50$, $\Delta t = 1/1200$, $\Omega = [0, 1]$, $p = -1.0$, $q = -0.001$ and $r = 1.0$. The initial data is $u(x, 0) = 0.1 \sin(2\pi x) + 0.01 \cos(4\pi x) + 0.06 \sin(4\pi x) + 0.02 \cos(10\pi x)$.

6 Conclusion

We have described how to design finite difference schemes which inherit properties (5) (and (8)) from PDEs in (2). The proposed method is easy, simple and applicable to many equations. Some examples which are derived through our proposed procedure are shown.

Since all discrete basic operators we use are symmetric in time, 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.

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 example in two-dimension, two space axes are orthogonal is shown in [8].

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Appendix Proof of Iteration of Summation by Parts

In this section we prove (32). For a matrix (of vector) A in general its transpose is denoted by A^{T}.

Lemma **5**

(97)
$$\delta^{\langle h\rangle} = \boldsymbol{e}^{\mathsf{T}} D^h\, \boldsymbol{e}$$

where

(98)
$$D \stackrel{\text{def}}{=} \begin{pmatrix} 0 & \delta^{+} \\ \delta^{-} & 0 \end{pmatrix},$$

(99)
$$\boldsymbol{e} \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Proof : This relation is trivial. $\square$

LEMMA **6**

$$(100) \qquad \sum_{k=0}^{N}{}'' \left\{ aDa' + (Da^{\mathsf{T}})^{\mathsf{T}} a' \right\} \Delta x = \frac{1}{2} \left[aAa' + (Aa^{\mathsf{T}})^{\mathsf{T}} a' \right]_{k=0}^{N}$$

where

$$(101) \qquad a \stackrel{\text{def}}{=} \begin{pmatrix} a_k & b_k \\ c_k & d_k \end{pmatrix},$$

$$(102) \qquad a' \stackrel{\text{def}}{=} \begin{pmatrix} a'_k & b'_k \\ c'_k & d'_k \end{pmatrix},$$

$$(103) \qquad A \stackrel{\text{def}}{=} \begin{pmatrix} 0 & s^+ \\ s^- & 0 \end{pmatrix}.$$

Proof : From (31) we obtain this equation. $\square$

LEMMA **7**

$$(104) \sum_{k=0}^{N}{}'' \left\{ aD^h a' \right\} \Delta x$$

$$= (-1)^{h'} \sum_{k=0}^{N}{}'' \left(D^{h'} a^{\mathsf{T}} \right)^{\mathsf{T}} \left(D^{h-h'} a' \right) \Delta x$$

$$+\frac{1}{2} \left[\sum_{l=1}^{h'} (-1)^{l-1} \left\{ \left(D^{l-1} a^{\mathsf{T}} \right)^{\mathsf{T}} \left(AD^{h-l} a' \right) + \left(AD^{l-1} a^{\mathsf{T}} \right)^{\mathsf{T}} \left(D^{h-l} a' \right) \right\} \right]_{k=0}^{N}$$

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

Proof : We obtain this equation from iterative application of (100) to LHS of this equation. $\square$

From this lemma and Lemma 5 we obtain the following equation.

$$(105) \qquad \sum_{k=0}^{N}{}'' f_k \delta^{\langle h \rangle} f_k \, \Delta x$$

$$= (-1)^{h'} \sum_{k=0}^{N}{}'' \left\{ \boldsymbol{e}^{\mathsf{T}} \left(D^{h'} f_k \right)^{\mathsf{T}} \left(D^{h-h'} f_k \right) \boldsymbol{e} \right\} \Delta x$$

$$+\frac{1}{2} \left[\sum_{l=1}^{h'} (-1)^{l-1} \left\{ \boldsymbol{e}^{\mathsf{T}} \left(D^{l-1} f_k \right)^{\mathsf{T}} \left(AD^{h-l} f_k \right) \boldsymbol{e} \right\} \right.$$

$$\left. + \sum_{l=1}^{h'} (-1)^{l-1} \left\{ \boldsymbol{e}^{\mathsf{T}} \left(AD^{l-1} f_k \right)^{\mathsf{T}} \left(D^{h-l} f_k \right) \boldsymbol{e} \right\} \right]_{k=0}^{N}$$

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

Substituting $h' = h/2$ into this equation we obtain (32) for even h. When h is odd, we obtain (32) by comparing this equation with $h' = (h-1)/2$ and the one with $h' = (h+1)/2$.