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Spatially Accurate Conservative or Dissipative Finite Difference Schemes Derived by the Discrete Variational Method ⋆

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Abstract

A method, called "the discrete variational method", has been recently presented by Furihata and Matsuo for designing finite difference schemes that inherit energy conservation or dissipation property from nonlinear partial differential equations (PDEs). In this paper the method is enhanced so that the derived schemes be highly accurate in space by introducing higher order spatial difference operators, including the so-called "spectral differentiation" operator. Applications to the KdV equation, and the cubic nonlinear Schrödinger equation are also presented.

Key words: finite difference method, pseudospectral method, energy conservation, energy dissipation, KdV equation, nonlinear Schrödinger equation

1 Introduction

In this paper we present an enhanced version of the discrete variational method for designing "spatially accurate" finite difference schemes that inherit energy conservation or dissipation property from PDEs.

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The discrete variational method was firstly proposed by Furihata[4] for the real dissipative partial differential equations(PDEs) of the form

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

and the real conservative PDEs of the form

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

where $G = G(u, u_x)$ is a function of real-valued functions u and $u_x = \partial u/\partial x$, and $\delta G/\delta u$ is the variational derivative of $G(u, u_x)$ for u. There, based on a newly invented concept "*discrete* variational derivative", which is a discrete analogue of the variational derivative, finite difference schemes are defined analogously to (1) or (2). And the defined schemes are shown to "inherit" the dissipation or conservation property. The method was then soon extended by Matsuo and Furihata[7] to the complex dissipative PDEs of the form

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \quad (t > 0, x \in [0, L]), \tag{3}$$

and the complex conservative PDEs of the form

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \quad (t > 0, x \in [0, L]), \tag{4}$$

where $\mathrm{i} = \sqrt{-1}$, u is a complex-valued function, $\overline{u}$ is the complex conjugate of u, and $\delta G/\delta \overline{u}$ is the complex variational derivative of $G(u, u_x)$ for $\overline{u}$. For both real and complex cases, the method has an additional advantage that the derived schemes shall keep the inherited properties even if the time mesh size changes in the time-evolution process. It enables us to use some appropriate time mesh size adaptive methods to reduce computational cost, or some linear acceleration methods to increase accuracy in time. Because of these properties and advantage, the derived schemes are expected to be numerically stable and yield solutions converging to PDE solutions, and sufficiently flexible to treat. In fact, the derived schemes were shown to be stable and convergent for the Cahn-Hilliard Equation[5], and for the nonlinear Schrödinger equation[7].

The accuracy of the derived schemes is, however, only $O(\Delta t^2, \Delta x^2)$, because the usual difference operators of $O(\Delta t^2)$ and $O(\Delta x^2)$ are used in the method (where Δt and Δx are time- and space-mesh sizes, respectively). It is sufficient for most problems, while sometimes more accuracy is demanded. In this paper, to meet this demand partially, we newly present an enhanced version of the method, by which we can derive *spatially* more accurate schemes for the problems which are under the periodic boundary condition:

$$\left.\frac{\partial^j u}{\partial x^j}\right|_{x=0} = \left.\frac{\partial^j u}{\partial x^j}\right|_{x=L}, \quad (j = 0, 1, \ldots, J), \tag{5}$$

where $J \geq 1$ is specific to each problems. To accomplish this, we utilize more accurate difference operators, including the so-called "spectral differentiation" operator.

This paper is organized as follows. In Section 2 we describe the discrete symbols we employ in this paper. In Section 3 we present the enhanced version of the discrete variational method for both real and complex PDEs. In Section 4 we present applications to the KdV equation and the cubic nonlinear Schrödinger equation. Section 5 is for conclusion.

2 Discrete Symbols and Formulas

In this section we describe the discrete symbols and the formulas employed in this paper.

We denote the numerical solution as

$$U_k^{(m)} \simeq u(k\Delta x, m\Delta t) \qquad (k \in \mathbb{Z}, m = 0, 1, 2, \cdots), \tag{6}$$

where $\Delta x = L/N$, and $\Delta t > 0$ are the mesh sizes in x, t, respectively. N is the number of the spatial grid points. The time step (m) is omitted unless indispensable. Corresponding to the continuous periodic boundary condition (5), we apply the discrete periodic boundary condition:

$$U_k = U_{k+\omega N}, \quad 0 \leq k \leq N-1, \omega \in \mathbb{Z}. \tag{7}$$

Next we introduce the 1st difference operator of $O(\Delta x^{2p})$ $(p = 1, 2, \ldots)$:

$$\delta_k^{\langle 1 \rangle, 2p} U_k = \sum_{j=-p}^{p} \frac{\alpha_{p,j} U_{k+j}}{\Delta x}. \tag{8}$$

The coefficients $\alpha_{p,j}$ are uniquely determined to gain optimal accuracy, and skew-symmetric, i.e. $\alpha_{p,j} = -\alpha_{p,-j}$ (see, for example, Fornberg [3]). When $p = 1$, it is reduced to the standard central difference operator: $\delta_k^{\langle 1 \rangle} U_k =$

$(U_{k+1}-U_{k-1})/2\Delta x$. And in the limit of $p\to\infty$, $\delta_k^{\langle 1\rangle,2p}$ becomes the so-called "spectral differentiation" operator:

$$\delta_k^{\langle 1\rangle,\infty}U_k=\left(F^{-1}\tilde{D}F\boldsymbol{U}\right)_k, \tag{9}$$

where $\boldsymbol{U}=(U_0,U_1,\ldots,U_{N-1})^{\mathrm{T}}$ and

$$F_{jk}\overset{\mathrm{d}}{\equiv}\frac{1}{N}\exp\left(-\frac{2\mathrm{i}\pi jk}{N}\right), \tag{10}$$

$$\tilde{D}\overset{\mathrm{d}}{\equiv}\mathrm{diag}\left\{0,\frac{2\pi\mathrm{i}}{L},\ldots,\frac{2\pi\mathrm{i}(\frac{N}{2}-1)}{L},0,-\frac{2\pi\mathrm{i}(\frac{N}{2}-1)}{L}),\ldots,-\frac{2\pi\mathrm{i}}{L}\right\}. \tag{11}$$

Thus the derived schemes below include a pseudospectral-like scheme as a special case.

With regard to the differentiation operator $\delta_k^{\langle 1\rangle,2p}$, the following "summation-by-part" holds, which is a discrete analogue of the integration-by-part formula. This formula is the most essential tool in our discrete variational method.

Lemma 1 (Summation-by-Part) *For any two N-periodic sequences U_k,V_k $(0\le k\le N-1)$,*

$$\sum_{k=0}^{N-1}(\delta_k^{\langle 1\rangle,2p}U_k)V_k\Delta x=-\sum_{k=0}^{N-1}U_k(\delta_k^{\langle 1\rangle,2p}V_k)\Delta x. \tag{12}$$

PROOF.

$$\begin{aligned}\sum_{k=0}^{N-1}\left(\delta_k^{\langle 1\rangle,2p}U_k\right)V_k\Delta x&=\sum_{k=0}^{N-1}\left(\sum_{j=-p}^{p}\alpha_{p,j}U_{k+j}\right)V_k\\&=\sum_{j=-p}^{p}\left(\sum_{k'=j}^{N-1+j}\alpha_{p,j}U_{k'}V_{k'-j}\right)\\&=\sum_{j=-p}^{p}\left(\sum_{k'=0}^{N-1}\alpha_{p,j}U_{k'}V_{k'-j}\right)\\&=-\sum_{j'=-p}^{p}\left(\sum_{k'=0}^{N-1}\alpha_{p,j'}U_{k'}V_{k'+j'}\right)\\&=-\sum_{k=0}^{N-1}U_k(\delta_k^{\langle 1\rangle,2p}V_k)\Delta x.\end{aligned} \tag{13}$$

The third equality is from the periodic boundary condition (7), and the fourth is from the skew-symmetry: $\alpha_{p,j}=-\alpha_{p,-j}$. ∎

3 The Discrete Variational Method with the Difference Operator $\delta_k^{\langle 1\rangle,2p}$

In this section we present the enhanced version of the discrete variational method for both real and complex PDEs. It is essentially based on the previously proposed discrete variational method[4,7], but it utilizes the highly accurate spatial difference operator $\delta_k^{\langle 1\rangle,2p}$ instead of the standard 2nd order accurate operator $\delta_k^{\langle 1\rangle}$. This modification is made possible by the summation-by-part formula with regard to $\delta_k^{\langle 1\rangle,2p}$, presented in the previous section.

3.1 For the real PDEs

3.1.1 Target equations and their properties

We here consider the real dissipative PDEs (1) and conservative PDEs (2) under the periodic boundary condition (5). And as in Furihata[4], for the sake of simplicity, we assume that $G(u, u_x)$ be of the form:

$$G(u, u_x) = \sum_{l=1}^{M} p_l(u) q_l(u_x), \tag{14}$$

where $M \in \mathbb{N}^+$, and $p_l, q_l : \mathbb{R} \to \mathbb{R}$ are differentiable functions. Most of the important applications are covered by this class of $G(u, u_x)$.

Under these settings, the dissipative PDEs (1) dissipate the "global energy" as follows.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u, u_x)\mathrm{d}x &= \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\mathrm{d}x \\
&= \int_0^L \frac{\delta G}{\delta u}(-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s}\frac{\delta G}{\delta u}\mathrm{d}x \\
&= -\int_0^L \left\{\left(\frac{\partial}{\partial x}\right)^{s}\frac{\delta G}{\delta u}\right\}^2 \mathrm{d}x \le 0.
\end{aligned} \tag{15}$$

In the third equality, the integration by part formula is repeatedly used. The difference terms at boundaries are dropped due to the periodicity (5). The Cahn-Hilliard equation, for example, is a real dissipative equation of this form (see, for example, Furihata[4]).

Similarly the conservative PDEs (2) conserves the global energy, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x = \int_0^L \frac{\delta G}{\delta u}\left(\frac{\partial}{\partial x}\right)^{2s+1}\left(\frac{\delta G}{\delta u}\right)\mathrm{d}x = 0. \tag{16}$$

The KdV equation,

$$u_t + uu_x + u_{xxx} = 0, \quad (t>0, x\in[0,L]), \tag{17}$$

is a real conservative equation of this form (a finite difference scheme for it will be given in Section 4).

3.1.2 Design of schemes

We firstly define the "discrete local energy" $G_{\mathrm{d}}(\boldsymbol{U})$ analogously to (14) as

$$G_{\mathrm{d}}(\boldsymbol{U})_k = \sum_{l=1}^{M} p_l(U_k) q_l(\delta_k^{\langle 1\rangle,2p} U_k). \tag{18}$$

For such a G_{d}, we consider the difference:

$$\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U})\Delta x - \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{V})\Delta x = \sum_{k=0}^{N-1} \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})}_k (U_k - V_k)\Delta x, \tag{19}$$

where

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})}_k \stackrel{\mathrm{d}}{\equiv} \frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})}_k - \delta_k^{\langle 1\rangle,2p}\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta(\boldsymbol{U},\boldsymbol{V})}_k\right), \tag{20}$$

and

$$\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})}_k = \sum_{l=1}^{M}\left\{\left(\frac{q_l(\delta_k^{\langle 1\rangle,2p}U_k) + q_l(\delta_k^{\langle 1\rangle,2p}V_k)}{2}\right)\left(\frac{p_l(U_k) - p_l(V_k)}{(U_k - V_k)}\right)\right\} \tag{21}$$

$$\frac{\partial G_{\mathrm{d}}}{\partial\delta(\boldsymbol{U},\boldsymbol{V})}_k = \sum_{l=1}^{M}\left\{\left(\frac{p_l(U_k) + p_l(V_k)}{2}\right)\left(\frac{q_l(\delta_k^{\langle 1\rangle,2p}U_k) - q_l(\delta_k^{\langle 1\rangle,2p}V_k)}{\delta_k^{\langle 1\rangle,2p}(U_k - V_k)}\right)\right\} \tag{22}$$

The difference (19) corresponds to the continuous variation calculation $\int_0^L G(u+\delta u, u_x+\delta u_x)\mathrm{d}x - \int_0^L G(u,u_x)\mathrm{d}x = \int_0^L \frac{\delta G}{\delta u}\delta u \mathrm{d}x + O(\delta u^2)$. The term $\delta G_{\mathrm{d}}/\delta(\boldsymbol{U},\boldsymbol{V}) : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}^N$ in the right hand side is a "discrete" version of the variational derivative $\delta G/\delta u$, and therefore we call it the "discrete variational derivative" of G_{d}. (Similarly $\partial G_{\mathrm{d}}/\partial(\boldsymbol{U},\boldsymbol{V}):\mathbb{R}^N\times\mathbb{R}^N\to\mathbb{R}^N$ corresponds to $\partial G/\partial u$, and $\partial G_{\mathrm{d}}/\partial\delta(\boldsymbol{U},\boldsymbol{V}):\mathbb{R}^N\times\mathbb{R}^N\to\mathbb{R}^N$ to $\partial G/\partial u_x$.) We omit the detail of the above calculation, but would much like to point out that the summation-by-part formula (12) is used.

With the discrete variational derivative, we then define the finite difference scheme for the real dissipative PDEs (1) by

$$\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}=(-1)^{s+1}\left(\delta_k^{\langle 1\rangle,2p}\right)^{2s}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}, \tag{23}$$

and for the real conservative PDEs (2) by

$$\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}=\left(\delta_k^{\langle 1\rangle,2p}\right)^{2s+1}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}. \tag{24}$$

The schemes dissipate or conserve the "discrete global energy" as follows.

Theorem 2 (Discrete energy dissipation) *The solution of the scheme (23) dissipates the discrete global energy $\sum_{k=0}^{N-1}G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x$, i.e.,*

$$\sum_{k=0}^{N-1}G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)})\Delta x\le\sum_{k=0}^{N-1}G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x,\quad(m=0,1,2,\ldots) \tag{25}$$

PROOF.

$$\begin{aligned}
&\frac{1}{\Delta t}\left(\sum_{k=0}^{N-1}G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)})\Delta x-\sum_{k=0}^{N-1}G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x\right)\\
&=\sum_{k=0}^{N-1}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\left(\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}\right)\Delta x\\
&=\sum_{k=0}^{N-1}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}(-1)^{s+1}\left(\delta_k^{\langle 1\rangle,2p}\right)^{2s}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right)\Delta x\\
&=-\sum_{k=0}^{N-1}\left\{\left(\delta_k^{\langle 1\rangle,2p}\right)^{2s}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right)\right\}^2\Delta x\\
&\le 0.
\end{aligned} \tag{26}$$

The second equality is from the definition of the scheme (23), and in the third equality the summation-by-part formula (12) is repeatedly used. ∎

Theorem 3 (Discrete energy conservation) *The solution of the scheme (24) conserves the discrete global energy* $\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x$*, i.e.,*

$$\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x = \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(0)})\Delta x, \quad (m = 1, 2, 3, \ldots) \tag{27}$$

PROOF.

$$\begin{aligned}
&\frac{1}{\Delta t}\left(\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)})\Delta x - \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x\right) \\
&= \sum_{k=0}^{N-1} \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right) \Delta x \\
&= \sum_{k=0}^{N-1} \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \left(\delta_k^{\langle 1\rangle, 2p}\right)^{2s+1} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}\right) \Delta x \\
&= (-1)^s \sum_{k=0}^{N-1} \left\{ \left(\delta_k^{\langle 1\rangle, 2p}\right)^{s} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}\right) \right. \\
&\qquad\qquad \left. \cdot \left(\delta_k^{\langle 1\rangle, 2p}\right)^{s+1} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}\right) \right\} \Delta x \\
&= 0.
\end{aligned} \tag{28}$$

The second equality is from the definition of the scheme (24). and in the third equality the summation-by-part formula (12) is repeatedly used. (Note that the equality $\sum_{k=0}^{N-1} U_k \delta_k^{\langle 1\rangle, 2p} U_k \Delta x = 0$ holds for any N-periodic sequence U_k, which can be easily obtained from (12) as a special case.) ∎

It is worth mentioning that the properties also hold even if Δt is changed during the time-evolution process (observe that the proofs concern only two consecutive time steps). So the derived schemes can be solved by some time mesh adaptive method to reduce computational cost, or some linear acceleration method to increase accuracy with regard to Δt (which is still only $O(\Delta t^2)$ in (23) and (24)).

Remark 4 In addition to the energy dissipation or conservation property, the schemes (23) and (24) have the "discrete mass" conservation property, i.e.,

$$\sum_{k=0}^{N-1} U_k^{(m)} \Delta x = \sum_{k=0}^{N-1} U_k^{(0)}, \quad (m = 1, 2, 3, \ldots), \tag{29}$$

which corresponds to the continuous "mass" conservation property:

$$\int_0^L u(t,x)\mathrm{d}x = \int_0^L u(0,x)\mathrm{d}x, \quad (t>0). \tag{30}$$

3.2 *For the complex PDEs*

3.2.1 *Target equations and their properties*

We here consider the complex dissipative PDEs (3) and conservative PDEs (4) under the periodic boundary condition (5). As in Matsuo and Furihata[7], we assume that the energy $G(u,u_x)$ takes the form

$$G(u,u_x) = \sum_{l=1}^{M} |p_l(u)|^{N_l^P} |q_l(u_x)|^{N_l^Q} \tag{31}$$

where $N_l^P, N_l^Q \in \{2,3,4,\ldots\}$, and $p_l, q_l : \mathbb{C} \to \mathbb{C}$ are assumed to be analytic functions which satisfy $p_l(\overline{u}) = \overline{p_l(u)}, q_l(\overline{u}) = \overline{q_l(u)}$ $(u \in \mathbb{C})$. Hereafter we abbreviate $|p_l(U_k)|^{N_l^P}$ as $P_l(U_k)$, and $|q_l(\delta_k^{\langle 1\rangle,2p} U_k)|^{N_l^Q}$ as $Q_l(U_k)$.

Under these settings, the dissipative PDEs (3) dissipate the global energy as follows.

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x &= \int_0^L \left\{ \frac{\delta G}{\delta u}\frac{\partial u}{\partial t} + \frac{\delta G}{\delta \overline{u}}\frac{\partial \overline{u}}{\partial t} \right\} \mathrm{d}x \\ &= -2\int_0^L \left| \frac{\delta G}{\delta u} \right|^2 \mathrm{d}x \le 0. \end{aligned} \tag{32}$$

The difference terms at boundaries are again dropped due to the periodicity (5). The real-coefficient Ginzburg-Landau equation and Newell-Whitehead equation, for example, are complex dissipative equations of this form (see, for example, [7]).

Similarly the conservative PDEs (4) conserve the global energy, i.e.,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x &= \int_0^L \left\{ \frac{\delta G}{\delta u}\frac{\partial u}{\partial t} + \frac{\delta G}{\delta \overline{u}}\frac{\partial \overline{u}}{\partial t} \right\} \mathrm{d}x \\ &= \int_0^L \left(-\mathrm{i}\left| \frac{\delta G}{\delta u} \right|^2 + \mathrm{i}\left| \frac{\delta G}{\delta u} \right|^2 \right) \mathrm{d}x = 0. \end{aligned} \tag{33}$$

The cubic nonlinear Schrödinger equation:

$$\mathrm{i}u_t = -u_{xx} - \gamma|u|^2 u, \quad (t > 0, x \in [0, L], \gamma \in \mathbb{R}), \tag{34}$$

is a complex conservative equation of this form (a finite difference scheme for it will be given in Section 4).

3.2.2 Design of schemes

We firstly define that the discrete energy $G_{\mathrm{d}}(\boldsymbol{U})$ analogously to (31) as

$$G_{\mathrm{d}}(\boldsymbol{U})_k = \sum_{l=1}^{M} |p_l(U_k)|^{N_l^P} |q_l(\delta_k^{\langle 1\rangle,2p} U_k)|^{N_l^Q}. \tag{35}$$

As in the real case, we consider the difference

$$\begin{aligned} &\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U})\Delta x - \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{V})\Delta x = \\ &\sum_{k=0}^{N-1} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})}_k (U_k - V_k) + \frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}_k (\overline{U_k - V_k}) \right) \Delta x, \end{aligned} \tag{36}$$

where

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})} \right)_k \overset{\mathrm{d}}{\equiv} \left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})} \right)_k - \delta_k^{\langle 1\rangle,2p} \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta(\boldsymbol{U},\boldsymbol{V})} \right)_k, \tag{37}$$

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})} \right)_k \overset{\mathrm{d}}{\equiv} \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})} \right)_k - \delta_k^{\langle 1\rangle,2p} \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})} \right)_k, \tag{38}$$

are the "complex discrete variational derivatives." In the above definition,

$$\begin{aligned} \left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})} \right)_k &\overset{\mathrm{d}}{\equiv} \sum_{l=1}^{M} \left(\frac{Q_l(U_k) + Q_l(V_k)}{2} \right) \left(\frac{p_l(U_k) - p_l(V_k)}{U_k - V_k} \right) \\ &\times f\left(N_l^P; p_l(U_k), p_l(V_k)\right), \end{aligned} \tag{39}$$

$$\begin{aligned} \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta(\boldsymbol{U},\boldsymbol{V})} \right)_k &\overset{\mathrm{d}}{\equiv} \sum_{l=1}^{M} \left(\frac{P_l(U_k) + P_l(V_k)}{2} \right) \\ &\times \left(\frac{q_l(\delta_k^{\langle 1\rangle,2p} U_k) - q_l(\delta_k^{\langle 1\rangle,2p} V_k)}{\delta_k^{\langle 1\rangle,2p} U_k - \delta_k^{\langle 1\rangle,2p} V_k} \right) f\left(N_l^Q; q_l(\delta_k^{\langle 1\rangle,2p} U_k), q_l(\delta_k^{\langle 1\rangle,2p} V_k)\right), \end{aligned} \tag{40}$$

and

$$f(n;z_1,z_2) \stackrel{\mathrm{d}}{\equiv} \begin{cases} \dfrac{\overline{z_1+z_2}}{2}(|z_1|^{n-2}+|z_1|^{n-4}|z_2|^2+\cdots+|z_2|^{n-2}), & n: \text{even}, \\ \dfrac{\overline{z_1+z_2}}{2}\dfrac{|z_1|^{n-1}+|z_1|^{n-2}|z_2|+\cdots+|z_2|^{n-1}}{|z_1|+|z_2|}, & n: \text{odd}. \end{cases} \tag{41}$$

With the complex discrete variational derivatives, we then define the finite difference scheme for the complex dissipative PDEs (3) by

$$\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t} = -\left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}},\overline{\boldsymbol{U}^{(m)}})}\right)_k, \tag{42}$$

and for the conservative PDEs (4) by

$$\mathrm{i}\left(\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}\right) = -\left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}},\overline{\boldsymbol{U}^{(m)}})}\right)_k. \tag{43}$$

The schemes dissipate or conserve the discrete global energy as follows.

Theorem 5 (Discrete energy dissipation) *The solution of the scheme (42) dissipates the discrete global energy $\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x$, i.e.,*

$$\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)})\Delta x \le \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x, \quad (m=0,1,2,\ldots) \tag{44}$$

PROOF.

$$\begin{aligned} &\frac{1}{\Delta t}\left(\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)})\Delta x - \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x\right) \\ &= \sum_{k=0}^{N-1}\left\{\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})}\right)_k \left(\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}\right)\right. \\ &\qquad\qquad \left. + \left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}},\overline{\boldsymbol{U}^{(m)}})}\right)_k \left(\overline{\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}}\right)\right\}\Delta x \\ &= -2\sum_{k=0}^{N-1}\left|\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})}\right)_k\right|^2 \Delta x \le 0. \end{aligned} \tag{45}$$

The second equality is from the definition of the scheme (42) and the fact that the complex (discrete) variational derivatives are complex conjugates of each other. ∎

Theorem 6 (Discrete energy conservation) *The solution of the scheme (24) conserves the discrete global energy* $\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x$, *i.e.,*

$$\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x = \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(0)})\Delta x, \quad (m = 1, 2, 3, \ldots) \tag{46}$$

PROOF.

$$\begin{aligned}
&\frac{1}{\Delta t}\left(\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m+1)})\Delta x - \sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x\right)\\
&= \sum_{k=0}^{N-1} \left\{ \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})}\right)_k \left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right)\right.\\
&\qquad\qquad \left. + \left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}})}\right)_k \left(\overline{\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}}\right)\right\} \Delta x\\
&= \sum_{k=0}^{N-1} \left\{ \mathrm{i}\left|\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})}\right)_k\right|^2 - \mathrm{i}\left|\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})}\right)_k\right|^2\right\} \Delta x = 0.
\end{aligned} \tag{47}$$

∎

3.3 Remark — design of linearly-implicit schemes

The derived schemes (23),(24), and (42),(43) are nonlinearly-implicit in general due to the nonlinearity in the PDEs, but we can also modify the enhanced method for designing *linearly*-implicit schemes using the idea described in Matsuo and Furihata[7] (see also Furihata and Matsuo[6]). We omit the details, but will present two examples in Section 4. The linearly-implicit schemes are expected to be more efficient than the nonlinearly-implicit ones, whose efficiency strongly depends on the implementation. It should be noted, however, the linearly-implicit schemes have a drawback instead that the energy dissipation or conservation property is kept only if Δt stays unchanged.

4 Applications

In this section we present some application examples. We pick up the KdV equation (17) for the real case, and the cubic nonlinear Schrödinger (NLS) equation (34) for the complex case.

Let us consider the KdV equation (17) under the periodic boundary condition (5). The KdV equation is a special case of the real conservative PDE (2) with $s = 0$, $G(u, u_x) = -u^3/6 + u_x^2/2$.

Up to present, many numerical studies have been done by various numerical methods. We refer the readers to Taha *et al.*[9] for a review. They concluded that the pseudospectral scheme (including the so-called "split-step" scheme) was most efficient so far by numerical experiments. As for energy-conserving schemes, Furihata[4] proposed one whose order of accuracy was $O(\Delta t^2, \Delta x^2)$. There seems to be, however, no higher order energy-conserving scheme in literature.

Now we would like to derive a scheme by the new method. Following the proposed procedure, we firstly define the discrete local energy as

$$G_{\mathrm{d}}(\boldsymbol{U})_k \stackrel{\mathrm{d}}{\equiv} -\frac{U_k^3}{6} + \frac{(\delta_k^{\langle 1\rangle,2p} U_k)^2}{2}. \tag{48}$$

Note that it can be decomposed as assumed in (18). Calculating mechanically the discrete variational derivative by (20), (21), and (22), we have

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})}_k = -\frac{U_k^2 + U_k V_k + V_k^2}{6} - \left(\delta_k^{\langle 1\rangle,2p}\right)^2 \left(\frac{U_k + V_k}{2}\right). \tag{49}$$

Then from (24) we obtain the finite difference scheme:

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = -\delta_k^{\langle 1\rangle,2p} \left\{ \frac{{U_k^{(m+1)}}^2 + U_k^{(m+1)} U_k^{(m)} + {U_k^{(m)}}^2}{6} + \left(\delta_k^{\langle 1\rangle,2p}\right)^2 \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2}\right) \right\} \tag{50}$$

For the solution of the scheme, the discrete energy conservation theorem 3 holds. Moreover, it conserves the discrete mass $\sum_{k=0}^{N-1} U_k^{(m)} \Delta x$ as noted in Remark 4. It also should be noted that, as mentioned in Section 2, the scheme can be pseudospectral-like in the limit of $p \to \infty$.

Remark 7 As noted in Section 3.3, we can also design a *linearly*-implicit scheme for the KdV equation. It becomes

$$\frac{U_k^{(m+3)} - U_k^{(m)}}{3\Delta t} = \\ - \delta_k^{\langle 1 \rangle, 2p} \left\{ \frac{U_k^{(m+2)} U_k^{(m+1)}}{2} + \left(\delta_k^{\langle 1 \rangle, 2p}\right)^2 \left(\frac{U_k^{(m+3)} + U_k^{(m)}}{2} \right) \right\}. \quad (51)$$

This scheme conserves the discrete global energy:

$$\sum_{k=0}^{N-1} \left(\frac{U_k^{(m+3)} U_k^{(m+2)} U_k^{(m+1)}}{6} \\ - \frac{\left|\delta_k^{\langle 1 \rangle, 2p} U_k^{(m+3)}\right|^2 + \left|\delta_k^{\langle 1 \rangle, 2p} U_k^{(m+2)}\right|^2 + \left|\delta_k^{\langle 1 \rangle, 2p} U_k^{(m+1)}\right|^2}{6} \right) \Delta x. \quad (52)$$

4.2 Finite Difference Schemes for the NLS Equation

Let us consider the cubic nonlinear Schrödinger (NLS) equation (34) under the periodic boundary condition (5). It is a special case of the complex conservative PDE (4) with $G(u, u_x) = -|u_x|^2 + \frac{\gamma}{2}|u|^4$.

Also for the NLS equation, there are many numerical studies. We refer the readers to Taha *et al.*[8] for a review, where the pseudospectral scheme is shown to be most efficient. There are many energy-conserving schemes as well[1,2]. But they are all of $O(\Delta t^2, \Delta x^2)$ and there seems to be no higher order energy-conserving scheme in literature.

To derive such a scheme, we follow the proposed procedure. We firstly define the discrete local energy as

$$G_{\mathrm{d}}(\boldsymbol{U})_k \overset{\mathrm{d}}{\equiv} -|\delta_k^{\langle 1 \rangle, 2p} U_k|^2 + \frac{\gamma}{2}|U_k|^4. \quad (53)$$

Note that it can be decomposed as assumed in (31). Calculating mechanically the complex discrete variational derivatives by (37), (38), and (39),(40), we have

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}})} \right)_k = (\delta_k^{\langle 1 \rangle, 2p})^2 \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right) \\ + \gamma \left(\frac{|U_k^{(m+1)}|^2 + |U_k^{(m)}|^2}{2} \right) \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right). \quad (54)$$

Then from (43) we obtain the finite difference scheme:

$$\mathrm{i}\left(\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}\right)=-(\delta_k^{\langle 1\rangle,2p})^2\left(\frac{U_k^{(m+1)}+U_k^{(m)}}{2}\right)$$
$$-\gamma\left(\frac{|U_k^{(m+1)}|^2+|U_k^{(m)}|^2}{2}\right)\left(\frac{U_k^{(m+1)}+U_k^{(m)}}{2}\right). \qquad (55)$$

The conservation theorem 6 holds. Moreover, the scheme conserves the discrete "probability": $\sum_{k=0}^{N-1}|\boldsymbol{U}^{(m)}|^2\Delta x$, which is a discrete analogue of the probability conservation law: $\int_0^L|u|^2\mathrm{d}x=\mathrm{const}$. With these properties the scheme is shown to be stable and L^2-convergent. The proofs are omitted for they are outside the scope of this paper.

We present some numerical examples. We compare three numerical schemes: (i) the scheme (55) with $p=\infty$ (i.e. a pseudospectral-like scheme), (ii) the scheme (55) with $p=1$ (which turns out to be identical to the Delfour scheme[1,7]), and (iii) the standard pseudospectral scheme which uses the 4th order Runge-Kutta method. The schemes (i) and (ii) are strictly conservative. We pick up the exact periodic solution with $\gamma=2$:

$$u(x,t)=\sqrt{\frac{\lambda+\alpha}{\gamma}}\,\mathrm{cn}[\sqrt{\alpha}(x-vt),k]\exp\left[\mathrm{i}\frac{v}{2}x-\mathrm{i}\left(\frac{v^2}{4}-\lambda\right)t\right], \qquad (56)$$

for numerical experiment. Here, $\mathrm{cn}(x,k)$ is the Jacobi elliptic function of modulus k. And $\alpha=\sqrt{2\gamma A+\lambda^2}$, $k=\sqrt{(\lambda+\alpha)/(2\alpha)}$, $L=4K(k)/\sqrt{\alpha}$ and $v=4\pi/L$. λ and A are constants, and can be chosen arbitrarily. The constants were taken as: $A=1.0\times10^{-5}$, and $\lambda=1$. (So, $\alpha\simeq1.00002$, $k\simeq0.999990$, $L\simeq28.5708$, and $v\simeq0.439832$). We carried out all numerical experiments in double-precision.

Firstly, we compare the accuracies of the numerical solutions. Table 1 shows the maximal errors at $t=T=10$. We denote the exact solution at $t=T$ by $\boldsymbol{u}=(u(T,x_0),u(T,x_1),\ldots,u(T,x_{N-1}))^{\mathrm{T}}$, and the numerical solution by $\boldsymbol{U}^{(M)}$ where $M=T/\Delta t$. The mark "(*)" means that the result is almost at the best order which can be attained with the value of Δx (i.e. the order can not be improved by decreasing the size of Δt). According to the marked result, we can confirm that the scheme (i) is spatially highly accurate as expected; the error decreases almost exponentially with regard to N, while the error by the scheme (ii) decreases only at the rate of $O(\Delta x^2)$. The superiority becomes far more significant as N grows. The scheme (iii) is spatially at the same order as (i), because it utilizes the same spectral differentiation method. The temporal accuracy of the scheme (i) is, however, still $O(\Delta t^2)$, which can be increased by utilizing some linear acceleration method with regard to Δt.

Table 1

Maximal errors at $T = 10$

Scheme	Δx (N)	Δt	$\|\boldsymbol{U}^{(M)} - \boldsymbol{u}\|_\infty$
(i)	0.4464 (64)	0.001	3.85×10^{-4} (*)
	0.2232 (128)	0.01	1.40×10^{-4}
		0.001	1.40×10^{-6}
		0.0001	1.92×10^{-8}
		0.00001	6.58×10^{-9} (*)
	0.1116 (256)	0.001	1.40×10^{-6}
		0.0001	1.40×10^{-8}
		0.00001	1.41×10^{-10}
		0.000001	1.08×10^{-12} (*)
(ii)	0.4464 (64)	0.001	5.00×10^{-1} (*)
	0.2232 (128)	0.001	1.14×10^{-1} (*)
	0.1116 (256)	0.001	2.80×10^{-2} (*)
(iii)	0.4464 (64)	0.01	3.84×10^{-4} (*)
	0.2232 (128)	0.001	8.01×10^{-9} (*)
	0.1116 (256)	0.0001	3.58×10^{-12} (*)

Secondly, we compare the errors of the conserved quantities. Table 2 shows the discrete global energy and the discrete probability at $t = 0$ and 1000. The discrete global energy is defined as $\sum_{k=0}^{N-1} G_{\mathrm{d}}(\boldsymbol{U}^{(m)})\Delta x$, where G_{d} is given by (53) with $p = \infty$ in (i) and (iii), and $p = 1$ in (ii). We set $\Delta t = 0.02$ and $\Delta x = 0.4464(N = 64)$. The underlined digits include errors. According to the result, the discrete global energy and probability are well preserved by the schemes (i) and (ii), where all errors are due to rounding errors. On the contrary, the scheme (iii) does not preserve them; moreover we observed that the discrete global energy monotonously decreases and the discrete probability monotonously increases.

Table 2

Discrete energy and probability at $t = 0$ and 1000

Scheme	t	global energy	probability
(i)	0	-1.13975589252432	3.99988723541072
	1000	$-1.1397558925243\underline{7}$	$3.9998872354107\underline{0}$
(ii)	0	-1.17654813106903	3.99988723541072
	1000	$-1.17654813106\underline{883}$	$3.9998872354107\underline{6}$
(iii)	0	-1.13975589252432	3.99988723541072
	1000	$-1.13975\underline{613138778}$	$3.999887\underline{61459249}$

As a result, we can conclude that the scheme (i) has the advantage of the scheme (ii), i.e. the spatial high accuracy, and also that of the scheme (iii), i.e. the conservation properties.

Remark 8 As noted in Section 3.3, we can also design a *linearly*-implicit scheme for the NLS equation. It becomes

$$\mathrm{i}\left(\frac{U_k^{(m+2)} - U_k^{(m)}}{2\Delta t}\right) = \\ -\left(\delta_k^{\langle 1\rangle,2p}\right)^2\left(\frac{U_k^{(m+2)} + U_k^{(m)}}{2}\right) - \gamma|U_k^{(m+1)}|^2\left(\frac{U_k^{(m+2)} + U_k^{(m)}}{2}\right). \quad (57)$$

This scheme conserves the discrete global energy:

$$\sum_{k=0}^{N-1}\left\{-\frac{\left|\delta_k^{\langle 1\rangle,2p}U_k^{(m+2)}\right|^2 + \left|\delta_k^{\langle 1\rangle,2p}U_k^{(m+1)}\right|^2}{2} \right. \\ \left. + \frac{\gamma}{2}\left(\frac{\left|U_k^{(m+2)}\right|^4 + \left|U_k^{(m+1)}\right|^4}{2}\right)\right\}\Delta x. \quad (58)$$

5 Conclusion

We presented an enhanced version of the discrete variational method for designing spatially accurate finite difference schemes, including pseudospectral-like schemes, that inherit energy dissipation or conservation property from

PDEs. The derived schemes keep an welcome feature; the energy dissipation or conservation property is kept even if time-mesh size is changed during the time evolution process. Because of this, the derived schemes can be solved by some time-mesh adaptive methods to reduce computational cost, or some linear acceleration methods to increase accuracy with regard to Δt.

We also presented conservative pseudospectral-like schemes for the KdV equation and for the NLS equation, together with some numerical experiments for the NLS equation, demonstrating that the scheme is highly accurate in space and strictly conservative aside from rounding errors.

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