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Abstract

A new method is proposed for designing Galerkin schemes that retain the energy dissipation or conservation properties of nonlinear evolution equations such as the Cahn-Hilliard equation, the Korteweg-de Vries equation, or the nonlinear Schrödinger equation. In particular, as a special case, dissipative or conservative finite-element schemes can be derived. The key device there is the new concept of discrete partial derivatives. As examples of the application of the present method, dissipative or conservative Galerkin schemes are presented for the three equations.

Key words: Galerkin method, finite-element method, conservation, dissipation, Nonlinear Schrödinger equation, Cahn-Hilliard equation, Korteweg-de Vries equation
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1 Introduction

In this paper, the numerical integration of partial differential equations (PDEs for short) which have some "energy" conservation or dissipation properties is considered. For example, the Cahn-Hilliard (CH) equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right), \qquad 0 < x < L,\ t > 0, \tag{1}$$

where $p < 0, q < 0, r > 0$, has the "energy" dissipation property

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

when appropriate boundary conditions are imposed. The Korteweg-de Vries (KdV) equation,

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{2}u^2 + \frac{\partial^2 u}{\partial x^2}\right), \qquad 0 < x < L,\ t > 0, \tag{2}$$

has the energy conservation property

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L \left(\frac{1}{6}u^3 - \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2\right) \mathrm{d}x = 0,$$

again, when appropriate boundary conditions are imposed. The nonlinear Schrödinger (NLS) equation,

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x} - \gamma |u|^{p-1}, \qquad 0 < x < L,\ t > 0, \tag{3}$$

where $\mathrm{i} = \sqrt{-1}$, $p = 3, 4, \ldots$, and $\gamma \in \mathbf{R}$, has the “energy” conservation property

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L \left(-\left|\frac{\partial u}{\partial x}\right|^2 + \frac{2\gamma}{p+1}|u|^{p+1}\right) \mathrm{d}x = 0, \qquad t > 0,$$

under appropriate boundary conditions.

It is widely accepted that numerical schemes which retain the dissipation or conservation properties of the PDEs are advantageous in that they often yield physically correct results and numerical stability [2]. We call such schemes “dissipative/conservative schemes” in this paper. In the literature, this area was first approached by the development of a number of specific schemes corresponding to specific problems; the interested reader may refer to [1,3,4,9,10] among others (see also references in [5,7]). A more unified method was then given in [5–8], by which dissipative or conservative *finite-difference* schemes can be constructed automatically for certain classes of dissipative/conservative PDEs. More specifically, this method targets dissipative/conservative PDEs which are defined using a variational derivative. In Furihata [5], real-valued equations of the form

$$\frac{\partial u}{\partial t} = (-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s} \frac{\delta G}{\delta u}, \qquad s = 0, 1, 2, \ldots \tag{4}$$

were considered, where $\delta G/\delta u$ is the variational derivative of $G(u, u_x)$ with respect to $u(x,t)$. Under appropriate boundary conditions, these PDEs becomes dissipative. For example, the CH equation belongs to this class with $s = 1$ and $G(u, u_x) = pu^2/2 + ru^4/4 - qu_x^2/2$ (where $u_x = \partial u/\partial x$). Furihata also targeted real-valued conservative PDEs of the form

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{2s-1} \frac{\delta G}{\delta u}, \qquad s = 1, 2, 3, \ldots. \tag{5}$$

The KdV equation is an example of this class with $s = 1$ and $G(u, u_x) = u^3/6 - {u_x}^2/2$. Later, Matsuo and Furihata [7] considered complex-valued conservative equations of the form

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \tag{6}$$

where $\delta G/\delta \overline{u}$ is a complex variational derivative, and $\bar{u}$ is the complex conjugate of u. An example of this class is the NLS equation. Dissipative PDEs of the form $\partial u/\partial t = -\delta G/\delta \overline{u}$, were also treated. The key step for the above studies was the introduction of the "discrete variational derivative," which is a rigorous discretization of the variational derivative. Using the discrete variational derivative, a finite-difference scheme is defined analogously to the original equation, so that the dissipation/conservation property is automatically retained. Due to this underlying idea, the method is now called the "discrete variational derivative method" (DVDM). The method does, however, suffer from drawbacks due to being based on the finite-difference method. Specifically, the use of non-uniform grids and application to two- or three-dimensional problems with complex domain structures are not straightforward.

As a natural solution to this difficulty, we here propose a new method for designing *Galerkin* schemes that retain energy dissipation or conservation property. We limit ourselves to spatially one-dimensional cases for brevity, which is still enough to illustrate our essential idea. The resulting Galerkin schemes include as a special case finite-element schemes, which are highly flexible at handling spatially complex structures. The finite-element schemes can be implemented only with cheap H^1-elements (this feature shall be important when this method is extended to two- or three-dimensional problems). To be more specific, our ideas are summarized as follows: In order for the dissipation/conservation property, we borrow the concept of discrete derivative from the DVDM. In the present study, however, we abandon the discrete *variational* derivative, which generally includes second-derivatives u_{xx} and thus would require C^1-elements, but newly introduce the concept of "discrete *partial* derivatives" instead. We also propose to introduce intermediate variables and to consider mixed formulations appropriately, in order to unfold the higher-order derivatives such as $(\partial/\partial x)^{2s}$ in (4).

This paper is organized as follows: In Section 2 the target equations are defined. Section 3 is devoted to the proposed Galerkin method, while in Section 4 several application examples are shown. Finally, Section 5 offers some concluding remarks.

2 Target equations

Target PDEs and their dissipation or conservation properties are summarized. The first class is that given by all real-valued PDEs of the form of equation (4):

$$\frac{\partial u}{\partial t} = (-1)^{s+1} \left(\frac{\partial}{\partial x}\right)^{2s} \frac{\delta G}{\delta u}, \qquad s = 0, 1, 2, \ldots. \tag{4}$$

As mentioned above, these PDEs are dissipative.

Proposition 1 (Dissipation property of (4)) *Let us assume that boundary conditions satisfy*

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_0^L = 0. \quad t > 0, \tag{7}$$

Let us also assume when $s \geq 1$ *that*

$$\left[\left(\frac{\partial^{j-1}}{\partial x^{j-1}}\frac{\delta G}{\delta u}\right)\left(\frac{\partial^{2s-j}}{\partial x^{2s-j}}\frac{\delta G}{\delta u}\right)\right]_0^L = 0, \quad t > 0, \ j = 1, \ldots, s. \tag{8}$$

Then solutions to the PDEs (4) satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u, u_x)\mathrm{d}x \leq 0, \qquad t > 0.$$

That is, the PDEs are dissipative.

A proof can be found in [5]. Throughout this paper we call $G(u, u_x)$ the "local energy," and $\int_0^L G(u, u_x)\mathrm{d}x$ the "global energy." As stated above, the CH equation (1) is a member of this class with $s = 1$ and $G(u, u_x) = pu^2/2 + ru^4/4 - q{u_x}^2/2$.

The second class is the real-valued conservative PDEs of the form of equation (5):

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{2s-1} \frac{\delta G}{\delta u}, \qquad s = 1, 2, 3, \ldots. \tag{5}$$

Proposition 2 (Conservation property of (5)) *Let us assume that boundary conditions satisfy (7) and*

$$\left[\left(\frac{\partial^{j-1}}{\partial x^{j-1}}\frac{\delta G}{\delta u}\right)\left(\frac{\partial^{2s-1-j}}{\partial x^{2s-1-j}}\frac{\delta G}{\delta u}\right)\right]_0^L = 0, \quad t > 0, \ j = 1, \ldots, s. \tag{9}$$

Then solutions to the PDEs (5) satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u, u_x)\mathrm{d}x = 0, \qquad t > 0.$$

That is, the PDEs are conservative.

The KdV equation (2) is an example of this class with $s = 1$ and $G(u, u_x) = u^3/6 - {u_x}^2/2$.

The third class of PDEs considered in this study are the complex-valued PDEs (6):

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}. \tag{6}$$

Proposition 3 (Conservation property of (6)) *Let us assume that boundary conditions satisfy*

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}+\frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u}}{\partial t}\right]_0^L=0. \tag{10}$$

Then solutions to the PDEs (6) satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x=0, \qquad t>0.$$

That is, these PDEs are conservative.

A proof is given in [7]. Upon setting $G(u,u_x)=-|u_x|^2+2\gamma|u|^{p+1}/(p+1)$, it can be seen that the NLS equation (3) is an example of this class of equations.

3 The new Galerkin method

In this section the new method for designing dissipative or conservative Galerkin schemes is presented for the PDEs (4), (5), and (6) separately.

3.1 Dissipative schemes for the real-valued PDEs (4)

We commence by introducing the concept of "discrete partial derivatives." Suppose that local energy is of the form

$$G(u,u_x)=\sum_{l=1}^{M} f_l(u)g_l(u_x), \tag{11}$$

where $M\in\{1,2,\ldots\}$, and f_l, g_l are real-valued functions. For example, the local energy of the CH equation (1) can be expressed in this form with $M=3, f_1(u)=pu^2/2, g_1(u_x)=1, f_2(u)=ru^4/4, g_2(u_x)=1, f_3(u)=1, g_3(u_x)=-q{u_x}^2/2$. Let us denote the Galerkin approximate solution by $u^{(m)}\simeq u(x,m\Delta t)$ (Δt is the time mesh size). Then "discrete partial derivatives" are defined as follows.

Definition 4 (Discrete partial derivatives) *We call the discrete quantities*

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}:\equiv\sum_{l=1}^{M}\left(\frac{f_l(u^{(m+1)})-f_l(u^{(m)})}{u^{(m+1)}-u^{(m)}}\right)\left(\frac{g_l(u_x^{(m+1)})+g_l(u_x^{(m)})}{2}\right), \tag{12}$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}:\equiv\sum_{l=1}^{M}\left(\frac{f_l(u^{(m+1)})+f_l(u^{(m)})}{2}\right)\left(\frac{g_l(u_x^{(m+1)})-g_l(u_x^{(m)})}{u_x^{(m+1)}-u_x^{(m)}}\right), \tag{13}$$

the "discrete partial derivatives," which corresponds to $\partial G/\partial u$ and $\partial G/\partial u_x$, respectively[1].

[1] Expressions similar to $(f(a)-f(b))/(a-b)$ should be interpreted as $f'(a)$ when $a=b$.

It can be easily verified that, corresponding to the continuous chain rule:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x = \int_0^L \left(\frac{\partial G}{\partial u}u_t + \frac{\partial G}{\partial u_x}u_{xt}\right)\mathrm{d}x,$$

the following discrete chain rule holds (hereafter $G(u^{(m)}, u_x^{(m)})$ is abbreviated as $G(u^{(m)})$ to save space.)

Theorem 5 (Discrete chain rule (real-valued case)) *Concerning the discrete partial derivatives (12) and (13), the following identity holds.*

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right)\mathrm{d}x = \int_0^L \left\{\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)\right.$$
$$\left. + \frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\left(\frac{u_x^{(m+1)}-u_x^{(m)}}{\Delta t}\right)\right\}\mathrm{d}x. \qquad (14)$$

Now we are in a position to describe our schemes for the equation (4). The simplest case $s = 0$ and general cases $s = 1, 2, \ldots$ are treated separately. Let us denote the trial space by S_1, and the test space by W_1. We also use the notation $(f, g) = \int_0^L fg\mathrm{d}x$, and its associated norm $\|\cdot\|_2$.

Scheme 1 (Galerkin scheme for $s = 0$) *Suppose $u^{(0)}(x)$ is given in S_1. Find $u^{(m)} \in S_1$ $(m = 1, 2, \ldots)$ such that, for any $v \in W_1$,*

$$\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}, v\right) = -\left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}, v\right) - \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}, v_x\right)$$
$$+ \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}v\right]_0^L. \qquad (15)$$

Because the discrete partial derivatives (12) and (13) do not include second derivatives, the scheme can be implemented using only H^1-elements, such as the standard piecewise linear function space. The scheme is dissipative in the following sense.

Theorem 6 (Dissipation property of Scheme 1) *Assume that boundary conditions and the trial and test spaces are set such that*

$$\left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)\right]_0^L = 0, \qquad (16)$$

and $(u^{(m+1)} - u^{(m)})/\Delta t \in W_1$ hold. Then Scheme 1 is dissipative in the sense that

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right)\mathrm{d}x \le 0, \qquad m = 0, 1, 2, \ldots.$$

PROOF.

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x$$
$$= \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, \frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, \frac{u_x^{(m+1)} - u_x^{(m)}}{\Delta t}\right)$$
$$= -\left\|\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right\|_2^2 + \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L \leq 0.$$

The first equality is by Theorem 5. The second one is shown by making use of expression (15) and the assumption $(u^{(m+1)} - u^{(m)})/\Delta t \in W_1$. The inequality is shown by the assumption (16). □

The assumption (16) corresponds to the condition (7). The assumption $(u^{(m+1)} - u^{(m)})/\Delta t \in W_1$ can be usually satisfied with natural choices of S_1 and W_1. For example, when the Dirichlet boundary conditions $u(0) = a,\ u(L) = b$ are imposed, it is natural to take $S_1 = \{u \mid u(0) = a,\ u(L) = b\}$ and $W_1 = \{v \mid v(0) = 0,\ v(L) = 0\}$. In this setting the assumption is satisfied.

Next we proceed to the general case $s \geq 1$. We first observe that by recursively introducing intermediate variables: $p_1 = -(p_2)_{xx}, \ldots, p_{s-1} = -(p_s)_{xx}$, and $p_s = \delta G/\delta u$, the original equation (4) can be rewritten as a system of equations $u_t = (p_s)_{xx}$, $p_{j-1} = -(p_j)_{xx}$ $(j \in J)$, and $p_s = \delta G/\delta u$, where the set $J = \{2, \ldots, s\}$ when $s \geq 2$ or $J = \emptyset$ when $s = 1$. This leads us to the following scheme. We assume the trial spaces $S_1, \ldots, S_{s+1}$, and test spaces $W_1, \ldots, W_{s+1}$ accordingly.

Scheme 2 (Galerkin scheme for $s \geq 1$) *Suppose that $u^{(0)}(x)$ is given in S_{s+1}. Find $u^{(m+1)} \in S_{s+1}$, $p_1^{(m+\frac{1}{2})} \in S_1$, $\ldots$, $p_s^{(m+\frac{1}{2})} \in S_s$ $(m = 0, 1, \ldots)$ such that, for any $v_1 \in W_1$, $\ldots$, $v_{s+1} \in W_{s+1}$,*

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) = -\left((p_1^{(m+\frac{1}{2})})_x, (v_1)_x\right) + \left[(p_1^{(m+\frac{1}{2})})_x v_1\right]_0^L, \tag{17}$$

$$\left(p_{j-1}^{(m+\frac{1}{2})}, v_j\right) = \left((p_j^{(m+\frac{1}{2})})_x, (v_j)_x\right) - \left[(p_j^{(m+\frac{1}{2})})_x v_j\right]_0^L \quad (j \in J), \tag{18}$$

$$\left(p_s^{(m+\frac{1}{2})}, v_{s+1}\right) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, v_{s+1}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_{s+1})_x\right) - \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v_{s+1}\right]_0^L. \tag{19}$$

The equation (18) is dropped when $J = \emptyset$. This scheme can be also implemented only with H^1-elements. The dissipation property is summarized in the next theorem.

Theorem 7 (Dissipation property of Scheme 2) *Assume that boundary conditions and the trial and test spaces are set such that (i) the condition (16) is satisfied; (ii) $\left[(p_j^{(m+\frac{1}{2})})_x \cdot p_{s+1-j}^{(m+\frac{1}{2})}\right]_0^L = 0$ $(j = 1, 2, \ldots, s)$; (iii) $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{s+1}$; and (iv) $W_j \supseteq S_{s+1-j}$ $(j = 1, 2, \ldots, s)$. Then Scheme 2 is* *dissipative in the sense that*

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x \le 0, \qquad m = 0, 1, 2, \ldots.$$

PROOF.

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x \\
&= \left(\frac{\partial G_\mathrm{d}}{\partial(u^{(m+1)}, u^{(m)})}, \frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) + \left(\frac{\partial G_\mathrm{d}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, \frac{u_x^{(m+1)} - u_x^{(m)}}{\Delta t}\right) \\
&= \left(p_s^{(m+\frac{1}{2})}, \frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) + \left[\frac{\partial G_\mathrm{d}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L \\
&= -\left((p_1^{(m+\frac{1}{2})})_x, (p_s^{(m+\frac{1}{2})})_x\right) + \left[(p_1^{(m+\frac{1}{2})})_x p_s^{(m+\frac{1}{2})}\right]_0^L.
\end{aligned}$$

The second equality is shown by using equation (19) with $v_{s+1} = (u^{(m+1)} - u^{(m)})/\Delta t$. The third equality is given by using equation (17) with $v_1 = p_s^{(m+\frac{1}{2})}$ and the assumption $S_s \subseteq W_1$. By repeatedly making use of equation (18) with $j = s, 2, s-1, 3, \ldots$ in this order, which is allowed by the assumption (iv), it can be seen that the right-hand side is equal to $-\|(p_{(s+1)/2}^{(m+\frac{1}{2})})_x\|_2^2$ when s is odd, or $-\|p_{s/2}^{(m+\frac{1}{2})}\|_2^2$ otherwise, and so the proof is complete. All the boundary terms vanish as a result of the boundary-condition assumptions. □

Remark 8 We can see the perfect matching between Proposition 1 and Theorem 7. As noted before, the assumption (16) corresponds to the condition (7). It can be also checked that the assumption (ii) in Theorem 7 exactly corresponds to the condition (8), since the latter can be rewritten as $[(p_j)_x \cdot p_{s+1-j}]_0^L = 0$ $(j = 1, \ldots, s)$ with the intermediate variables p_j.

3.2 Conservative schemes for the real-valued PDEs (5)

Conservative schemes for the PDEs (5) are proposed using the discrete partial derivatives introduced in the previous section. The simplest case $s = 1$ and general cases $s = 2, 3, \ldots$ are treated separately. Let $S_1, \ldots, S_{s+1}$ be trial spaces, and $W_1, \ldots, W_{s+1}$ be test spaces.

Scheme 3 (Galerkin scheme for $s = 1$) *Suppose that $u^{(0)}(x)$ is given in S_2. Find $u^{(m+1)} \in S_2$, $p_1^{(m+\frac{1}{2})} \in S_1$ such that, for any $v_1 \in W_1$, $v_2 \in W_2$,*

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) = \left((p_1^{(m+\frac{1}{2})})_x, v_1\right) \tag{20}$$

$$\begin{aligned}
\left(p_1^{(m+\frac{1}{2})}, v_2\right) &= \left(\frac{\partial G_\mathrm{d}}{\partial(u^{(m+1)}, u^{(m)})}, v_2\right) + \left(\frac{\partial G_\mathrm{d}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_2)_x\right) \\
&\quad - \left[\frac{\partial G_\mathrm{d}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v_2\right]_0^L.
\end{aligned} \tag{21}$$

Theorem 9 (Conservation property of Scheme 3) *Assume that boundary conditions and the trial and test spaces are set such that (i) the condition (16) is satisfied; (ii)* $\left[(p_1^{(m+\frac{1}{2})})^2\right]_0^L = 0$*; (iii)* $(u^{(m+1)} - u^{(m)})/\Delta t \in W_2$*; and (iv)* $S_1 \subseteq W_1$*. Then Scheme 3 is conservative in the sense that*

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x = 0, \qquad m = 0, 1, 2, \ldots.$$

PROOF.

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x \\
&= \left(p_1^{(m+\frac{1}{2})}, \frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) + \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L \\
&= \left((p_1^{(m+\frac{1}{2})})_x, p_1^{(m+\frac{1}{2})}\right) = 0.
\end{aligned}$$

The first equality is shown by using equation (21) with $v_2 = (u^{(m+1)} - u^{(m)})/\Delta t$, while the second equality is given by using equation (20) with $v_1 = p_1^{(m+\frac{1}{2})}$ and the assumption $S_1 \subseteq W_1$. The last equality is from the assumption (ii). □

In order to describe the scheme for $s \geq 2$, let us define the set $J = \{2, \ldots, s\} \setminus \{n+1\}$ when $s = 2n$ $(n = 1, 2, \ldots)$, or $J = \{2, \ldots, s\} \setminus \{n\}$ when $s = 2n - 1$ $(n = 2, 3, \ldots)$.

Scheme 4 (Galerkin scheme for $s \geq 2$) *Suppose that* $u^{(0)}(x)$ *is given in* S_{s+1}*. Find* $u^{(m+1)} \in S_{s+1}$, $p_1^{(m+\frac{1}{2})} \in S_1$, $\ldots$, $p_s^{(m+\frac{1}{2})} \in S_s$ $(m = 0, 1, \ldots)$ *such that, for any* $v_1 \in W_1$, $\ldots$, $v_{s+1} \in W_{s+1}$,

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) = -\left((p_1^{(m+\frac{1}{2})})_x, (v_1)_x\right) + \left[(p_1^{(m+\frac{1}{2})})_x v_1\right]_0^L, \tag{22}$$

$$\left(p_{j-1}^{(m+\frac{1}{2})}, v_j\right) = -\left((p_j^{(m+\frac{1}{2})})_x, (v_j)_x\right) + \left[(p_j^{(m+\frac{1}{2})})_x v_j\right]_0^L \quad (j \in J), \tag{23}$$

$$\left(p_n^{(m+\frac{1}{2})}, (v_{n+1})_x\right) = \left((p_{n+1}^{(m+\frac{1}{2})})_x, (v_{n+1})_x\right) \quad (\textit{when } s = 2n), \tag{24}$$

$$\left(p_{n-1}^{(m+\frac{1}{2})}, v_n\right) = \left((p_n^{(m+\frac{1}{2})})_x, v_n\right) \quad (\textit{when } s = 2n-1), \tag{25}$$

$$\begin{aligned}
\left(p_s^{(m+\frac{1}{2})}, v_{s+1}\right) &= \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, v_{s+1}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_{s+1})_x\right) \\
&\quad - \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v_{s+1}\right]_0^L.
\end{aligned} \tag{26}$$

The equation (23) is dropped when $J = \emptyset$. The conservation property is summarized in the next theorem.

Theorem 10 (Conservation property of Scheme 4) *Assume that boundary conditions and trial and test spaces are set such that (i) the condition*

(16) is satisfied; (ii) $\left[(p_n^{(m+\frac{1}{2})})^2\right]_0^L = 0$ *and* $\left[(p_j^{(m+\frac{1}{2})})_x p_{s+1-j}^{(m+\frac{1}{2})}\right]_0^L = 0$ $(j \in J)$; *(iii)* $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{s+1}$; *and (iv)* $W_j \supseteq S_{s+1-j}$ $(j = 1, \ldots, s)$. *Then Scheme 3 is conservative in the sense that*

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x = 0, \qquad m = 0, 1, 2, \ldots.$$

PROOF. The proof is similar to Theorem 7.

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x = -\left((p_1^{(m+\frac{1}{2})})_x, (p_s^{(m+\frac{1}{2})})_x\right)$$
$$= \begin{cases} -\left((p_n^{(m+\frac{1}{2})})_x, (p_{n+1}^{(m+\frac{1}{2})})_x\right) & \text{(when } s = 2n\text{)}, \\ \left(p_{n-1}^{(m+\frac{1}{2})}, p_n^{(m+\frac{1}{2})}\right) & \text{(when } s = 2n-1\text{)}, \end{cases}$$
$$= (-1)^{s+1}\left(p_n^{(m+\frac{1}{2})}, (p_n^{(m+\frac{1}{2})})_x\right) = 0.$$

In the second equality the equation (23) is repeatedly used. The third equality is either from (24) or (25). □

Remark 11 The assumptions in Theorem 10 exactly correspond to those in Proposition 2, which can be checked similarly to Remark 8.

3.3 Conservative schemes for the complex-valued PDEs (6)

Before defining schemes, we first introduce complex versions of the discrete partial derivatives. Suppose that the local energy is again of the form of equation (11), but that f_l and g_l are real-valued functions of a *complex-valued* function $u(x,t)$, which satisfy $f_l(u) = f_l(\bar{u})$, and $g_l(u_x) = g_l(\bar{u}_x)$. Throughout this section, we use the notation $(f, g) = \int_0^L \overline{f} g \mathrm{d}x$. Then the complex discrete partial derivatives are defined as follows:

Definition 12 (Complex discrete partial derivatives) *We call the discrete quantities*

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})} :\equiv \sum_{l=1}^{M}\left(\frac{f_l(u^{(m+1)}) - f_l(u^{(m)})}{|u^{(m+1)}|^2 - |u^{(m)}|^2}\right)\left(\overline{\frac{u^{(m+1)} + u^{(m)}}{2}}\right) \times \left(\frac{g_l(u_x^{(m+1)}) + g_l(u_x^{(m)})}{2}\right), \tag{27}$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} :\equiv \sum_{l=1}^{M}\left(\frac{f_l(u^{(m+1)}) + f_l(u^{(m)})}{2}\right)\left(\frac{g_l(u_x^{(m+1)}) - g_l(u_x^{(m)})}{\left|u_x^{(m+1)}\right|^2 - \left|u_x^{(m)}\right|^2}\right) \times \left(\overline{\frac{u_x^{(m+1)} + u_x^{(m)}}{2}}\right), \tag{28}$$

which correspond to $\partial G/\partial u$ *and* $\partial G/\partial u_x$ *respectively, "complex discrete partial derivatives."*

Note that the complex discrete partial derivatives satisfy

$$\overline{\left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}\right)}=\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u^{(m+1)}},\overline{u^{(m)}})},\qquad \overline{\left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\right)}=\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}},\overline{u_x^{(m)}})}.$$

The following identity holds concerning the complex partial derivatives.

Theorem 13 (Discrete chain rule (complex-valued case))

$$\frac{1}{\Delta t}\int_0^L\left(G(u^{(m+1)})-G(u^{(m)})\right)\mathrm{d}x=\int_0^L\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)\mathrm{d}x$$
$$+\int_0^L\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\left(\frac{u_x^{(m+1)}-u_x^{(m)}}{\Delta t}\right)\mathrm{d}x+(\mathrm{c.c.}),$$

where (c.c.) *denotes the complex conjugates of the preceding terms.*

Making use of the complex discrete partial derivatives, a conservative scheme for the PDEs (5) is proposed as follows:

Scheme 5 (Galerkin scheme for the PDEs (5)) *Suppose that* $u^{(0)}(x)$ *is given in* S_1*. Find* $u^{(m)}\in S_1$ $(m=1,2,\ldots)$ *such that, for any* $v\in W_1$,

$$\mathrm{i}\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t},v\right)=-\left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u^{(m+1)}},\overline{u^{(m)}})},v\right)-\left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}},\overline{u_x^{(m)}})},v_x\right)$$
$$+\left[\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}},\overline{u_x^{(m)}})}v\right]_0^L.$$

Theorem 14 (Conservation property of Scheme 5) *Assume that boundary conditions are imposed so that*

$$\left[\left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\right)\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)+(\mathrm{c.c.})\right]_0^L=0,$$

and $(u^{(m+1)}-u^{(m)})/\Delta t\in W_1$*. Then Scheme 5 is conservative in the sense that*

$$\frac{1}{\Delta t}\int_0^L\left(G(u^{(m+1)})-G(u^{(m)})\right)\mathrm{d}x=0,\qquad m=0,1,2,\ldots.$$

PROOF.

$$\begin{aligned}&\frac{1}{\Delta t}\int_0^L\left(G(u^{(m+1)})-G(u^{(m)})\right)\mathrm{d}x\\&=\left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u^{(m+1)}},\overline{u^{(m)}})},\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)+\left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}},\overline{u_x^{(m)}})},\frac{u_x^{(m+1)}-u_x^{(m)}}{\Delta t}\right)+(\mathrm{c.c.})\\&=-\mathrm{i}\left\|\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right\|_2^2+\left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)\right]_0^L+(\mathrm{c.c.})\\&=0.\end{aligned}$$

□

4 Application examples

Application examples for the Cahn-Hilliard equation (1), the KdV equation (2), and the nonlinear Schrödinger equation (3) are presented. Suppose that the interval $[0, L]$ is partitioned appropriately, and let $S_h \in H^1(0, L)$ be, for example, the piecewise linear function space over the grid.

4.1 The Cahn-Hilliard equation

The CH equation (1) is an example of equation (4) with $s = 1$ and $G(u, u_x) = pu^2/2 + ru^4/4 - q{u_x}^2/2$, which is usually solved subject to the boundary conditions

$$u_x = 0 \quad \text{and} \quad \frac{\partial}{\partial x}\left(\frac{\delta G}{\delta u}\right) = 0 \qquad \text{at } x = 0, L. \tag{29}$$

Motivated by nature of the boundary conditions, let us set the trial spaces as $S_1, S_2 = \{v \mid v \in S_h,\ v_x(0) = v_x(L) = 0\}$, and the test spaces as $W_1, W_2 = S_h$. Then Scheme 2 reads as follows: find $u^{(m)} \in S_2$ and $p_1^{(m+\frac{1}{2})} \in S_1$ such that, for all $v_1 \in W_1$ and $v_2 \in W_2$,

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) = -\left((p_1^{(m+\frac{1}{2})})_x, (v_1)_x\right), \tag{30}$$

$$\left(p_1^{(m+\frac{1}{2})}, v_2\right) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, v_2\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_2)_x\right) \tag{31}$$

hold, where the terms

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})} = p\left(\frac{u^{(m+1)} + u^{(m)}}{2}\right) + r\left(\frac{(u^{(m+1)})^2 + (u^{(m)})^2}{2}\right)\left(\frac{u^{(m+1)} + u^{(m)}}{2}\right), \tag{32}$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} = q\left(\frac{u_x^{(m+1)} + u_x^{(m)}}{2}\right), \tag{33}$$

are obtained from definitions (12) and (13). Note that the boundary term $[(p_1^{(m+\frac{1}{2})})_x v_1]_0^L$ which should appear in equation (30) and also the $[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v_2]_0^L$ term in (31) vanish, because $(p_1^{(m+\frac{1}{2})})_x = u_x^{(m+1)} = u_x^{(m)} = 0$ at $x = 0, L$. It is easily checked that all the assumptions in Theorem 7 are satisfied, and thus the scheme is dissipative. This scheme coincides with the Du-Nicolaides scheme [4], except in the fact that Du and Nicolaides discussed this scheme only with (unphysical) zero Dirichlet boundary conditions.

Remark 15 In practice, the trial spaces can be taken as $S_1 = S_2 = S_h$ as in the standard elliptic problems. Then the boundary conditions (29) are automatically recovered as the natural boundary conditions from the equations (30) and (31).

Remark 16 The scheme has an additional conservation law:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L \frac{u^{(m+1)}-u^{(m)}}{\Delta t}\mathrm{d}x = 0, \qquad m = 0,1,2,\ldots, \tag{34}$$

which can be easily seen from the equation (17) with $v_1 = 1$.

4.2 The Korteweg-de Vries equation

The KdV equation (2) is an example of equation (5) with $s = 1$ and $G(u,u_x) = u^3/6 - {u_x}^2/2$. The periodic boundary conditions are assumed:

$$u(0,t) = u(L,t),\ u_x(0,t) = u_x(0,L), \qquad t > 0. \tag{35}$$

Let us select the trial and test spaces $S_1 = S_2 = W_1 = W_2 = \{v \mid v \in S_h,\ v(0) = v(L), v_x(0) = v_x(L)\}$. (Strictly speaking, we consider the L-periodic problem on $x \in (-\infty,\infty)$, and slightly staggered L-periodic grid which does not have nodes on $x = 0, L$, in order to avoid the ambiguity of u_x at $x = 0, L$.) Then Scheme 3 reads as follows: find $u^{(m)} \in S_2$ and $p_1^{(m+\frac{1}{2})} \in S_1$ such that, for all $v_1 \in W_1$ and $v_2 \in W_2$,

$$\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}, v_1\right) = \left((p_1^{(m+\frac{1}{2})})_x, v_1\right), \tag{36}$$

$$\left(p_1^{(m+\frac{1}{2})}, v_2\right) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}, v_2\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}, (v_2)_x\right) \tag{37}$$

hold, where

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})} = \frac{(u^{(m+1)})^2 + u^{(m+1)}u^{(m)} + (u^{(m)})^2}{6}, \tag{38}$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})} = -\frac{u_x^{(m+1)} + u_x^{(m)}}{2}, \tag{39}$$

are obtained from definitions (12) and (13). The boundary term appearing in (21) vanishes due to the periodicity of S_1 and W_1. Due to the periodicity of S_1, the assumption $[(p_1^{(m+\frac{1}{2})})^2]_0^L = 0$ is satisfied. The periodicity also implies that condition (16) is satisfied, thus all the assumptions in Theorem 9 are satisfied, and hence the scheme is conservative. To the best of our knowledge, this scheme seems new.

Remark 17 The scheme also has the additional conservation law (34). Set $v_1 = 1$ in the equation (20).

4.3 The nonliear Schrödinger equation

Let us consider the NLS equation (3) under the periodic boundary condition (35). This is an example of equation (5) with $G(u,u_x) = -|u_x|^2 + 2\gamma|u|^{p+1}/(p+1)$. Let us select the trial and test spaces $S_1 = W_1 = \{v \mid v \in S_h,\ v(0) =$

$v(L), v_x(0) = v_x(L)\}$. Then Scheme 5 becomes: find $u \in S_1$ such that, for all $v \in W_1$,

$$\mathrm{i}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v\right) = -\left(\frac{\partial G_\mathrm{d}}{\partial(\overline{u^{(m+1)}}, \overline{u^{(m)}})}, v\right) - \left(\frac{\partial G_\mathrm{d}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})}, v_x\right),$$

where the terms

$$\frac{\partial G_\mathrm{d}}{\partial(\overline{u^{(m+1)}}, \overline{u^{(m)}})} = \gamma\left(\frac{|u^{(m+1)}|^{p+1} - |u^{(m)}|^{p+1}}{|u^{(m+1)}|^2 - |u^{(m)}|^2}\right)\left(\frac{u^{(m+1)} + u^{(m)}}{2}\right), \tag{40}$$

$$\frac{\partial G_\mathrm{d}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})} = -\frac{u_x^{(m+1)} + u_x^{(m)}}{2}, \tag{41}$$

are obtained from definitions (27) and (28). The boundary term appearing in Scheme 5 vanishes due to the periodicity of S_1 and W_1. The periodicity also implies that condition (16) is satisfied, and thus the conservation property follows from Theorem 14. It may be noted that this scheme is simply the Akrivis-Dougalis-Karakashian scheme [1].

5 Concluding remarks

In this paper, a new method for designing dissipative/conservative Galerkin (or finite-element) schemes has been proposed. The resulting schemes by the method can be implemented only with cheap H^1 elements. Though we limited ourselves to spatially one-dimensional cases in this paper, the essential idea must be also valid in two- or three-dimensional cases. In such circumstances, however, more careful considerations on boundary and spatial integrations are required (note that all the spatial integrations should be done in machine accuracy in order for the strict dissipation or conservation). These issues will be discussed elsewhere in the near future.

As application examples, three schemes for the CH, KdV, and NLS equations have been presented. The schemes for the CH and NLS coincided with the novel schemes in the literature whose theoretical aspects are well-known. The scheme for the KdV seems new, and we are now investigating the scheme both experimentally and theoretically. We are also trying to apply the method to other dissipative/conservative PDEs. These results will be reported as soon as it is ready.

Finally, it is worth mentioning that the time mesh size can be changed adaptively in actual computation without destroying the strict dissipation or conservation property. It can be easily seen in each dissipation or conservation theorem. This feature can help reducing overall computational costs.

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