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Dissipative/conservative Galerkin schemes with discrete derivative for partial differential equations

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Abstract

A new method is proposed for designing Galerkin schemes that retain the energy dissipation or conservation properties of nonlinear partial differential equations such as the Cahn-Hilliard equation or the nonlinear Schrödinger equation. In particular, as a special case, dissipative or conservative finite-element schemes can be derived. The method is obtained by extending the existing "discrete variational derivative method," which was originally constructed on the finite-difference method. As examples of the application of the present method, it is shown that several dissipative/conservative Galerkin schemes in the literature can be systematically derived.

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 nonlinear Schrödinger (NLS) equation,

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

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

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

again, when appropriate boundary conditions are imposed.

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 [3]. We call such schemes "dissipative/conservative schemes"

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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, 2, 4, 6, 11] among others (see also references in [5, 8]).

A more unified method was then given in [5, 7, 8, 9], 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

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

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 $u_t = (\partial/\partial x)^{2s+1}\delta G/\delta u$ ($s = 0, 1, 2, \ldots$.). Later, Matsuo and Furihata [8] considered complex-valued conservative equations of the form

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \tag{4}$$

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. One natural way to circumvent this difficulty is to use instead the Galerkin approach, in particular the finite-element framework, which is more flexible at handling complex spatial structures.

The aim of this paper is to present a Galerkin dissipative/conservative method by extending the finite-difference DVDM. We limit ourselves to spatially one-dimensional cases for brevity. First, a natural Galerkin translation of the finite-difference DVDM is introduced, which unfortunately turns out to be impractical because it requires sufficiently smooth, i.e. expensive, basis functions. An improved method is then presented, which can be fully implemented by using only cheap H^1 elements. In this improvement, two key devices are important: The first device is the introduction of the concept of a "discrete *partial* derivative," which replaces the discrete *variational* derivative. The second device is the appropriate use of intermediate variables. This is necessary in order to treat the higher-order derivatives that appear due to the $(\partial/\partial x)^{2s}$ operator in equation (3).

This paper is organized as follows: In Section 2 the target equations are defined, while in Section 3 the natural Galerkin translation of the finite-difference DVDM is presented and its limitations are discussed. Section 4 is devoted to the improved, practical Galerkin method, while in Section 5 it is shown that several novel dissipative/conservative finite-element schemes in the literature can be derived by the proposed method. Finally, Section 6 offers some concluding remarks.

2 Target equations

In this paper, two classes of PDEs are considered. The first class is that given by all real-valued PDEs of the form of equation (3):

$$\frac{\partial u}{\partial t} = (-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s}\frac{\delta G}{\delta u}, \qquad s = 0, 1, 2, \dots. \tag{3}$$

As mentioned above, these PDEs are dissipative.

Proposition 2.1 (Dissipation property of (3)). *Let us assume that boundary conditions satisfy*

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_0^L = 0, \quad t > 0, \tag{5}$$

and

$$\left[\left(\frac{\partial^{j-1}}{\partial x^{j-1}}\frac{\delta G}{\delta u}\right)\left(\frac{\partial^{2s-j}}{\partial x^{2s-j}}\frac{\delta G}{\delta u}\right)\right]_0^L = 0, \quad t > 0,\ j = 1, \dots, s. \tag{6}$$

Then solutions to the PDEs (3) satisfy

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

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 $G(u, u_x) = pu^2/2 + ru^4/4 - qu_x^2/2$.

The second class of PDEs considered in this study are the complex-valued PDEs (4):

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}. \tag{4}$$

Proposition 2.2 (Conservation property of (4)). *Let us assume that boundary conditions satisfy*

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

Then solutions to the PDEs (4) 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 [8]. Upon setting $G(u, u_x) = -|u_x|^2 + 2\gamma|u|^{p+1}/(p+1)$, it can be seen that the NLS equation (2) is an example of this class of equations.

3 A Galerkin translation of the finite-difference DVDM

To facilitate an understanding of what follows, first, the essential idea of the DVDM is summarized. A natural Galerkin translation of the finite-difference DVDM is then presented and discussed.

3.1 Outline of the finite difference DVDM

Let us consider the PDEs (3) with $s = 0$,

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta u}. \tag{8}$$

Simply differentiating the global energy $\int_0^L G\,\mathrm{d}x$, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u, u_x)\mathrm{d}x = \int_0^L \frac{\delta G}{\delta u} u_t \mathrm{d}x + \left[\frac{\partial G}{\partial u_x} u_t\right]_0^L = -\int_0^L {u_t}^2 \mathrm{d}x + \left[\frac{\partial G}{\partial u_x} u_t\right]_0^L. \tag{9}$$

Thus if boundary conditions are imposed on the target equation such that the boundary term $[\cdot]_0^L$ is eliminated (for example, the Dirichlet condition $u_t = 0$ or periodic boundary conditions), the PDE is dissipative. Notice that the variational derivative plays a central role in the above calculation, and the concrete form of the local energy $G(u, u_x)$ is not required.

The DVDM takes full advantage of this observation. It supposes the following finite-difference analogue of (9):

$$\frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x =$$
$$\sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}\left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right)\Delta x + B_1(U_k^{(m+1)}, U_k^{(m)}), \tag{10}$$

where $\sum_{k=0}^{N}{}''$ is the trapezoidal rule, $U_k^{(m)} \simeq u(k\Delta x, m\Delta t)$ (and its vector notation $\boldsymbol{U}^{(m)}$) is the finite-difference solution, $G_{\mathrm{d},k}$ is discrete local energy, and $B_1(\cdot,\cdot)$ is the discrete boundary term corresponding to $\left[\frac{\partial G}{\partial u_x} u_t\right]_0^L$ in (9). Further details may be found in [5, 8]. The symbol $\delta G_{\mathrm{d}}/\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k$ is the discrete quantity which corresponds to the continuous variational derivative $\delta G/\delta u$, and thus is called the "discrete variational derivative." Under certain assumptions regarding the local energy, we can find the discrete variational derivative that satisfies the discrete variation identity (10). A finite-difference scheme can then be defined using this derivative,

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = -\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}, \tag{11}$$

analogously to the continuous equation (8). With this approach, the discrete dissipation property is guaranteed as follows:

$$\begin{aligned}
&\frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x \\
&= \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}\Delta x + B_1(U_k^{(m+1)},U_k^{(m)}) \\
&= -\sum_{k=0}^{N}{}'' \left(\frac{U_k^{(m+1)}-U_k^{(m)}}{\Delta t}\right)^2 \Delta x + B_1(U_k^{(m+1)},U_k^{(m)}).
\end{aligned} \tag{12}$$

The first equality holds by applying equation (10), and the second one by applying equation (11). If the boundary term $B_1(\cdot,\cdot)$ vanishes in light of the discrete boundary condition, the right-hand side is non-positive, which ensures the desired dissipativity. Notice that equation (12) is completely analogous to the continuous case given in equation (9).

3.2 A natural Galerkin translation

Let us try to exactly follow the above procedure within a Galerkin framework. In order to give rigorous definitions, suppose that local energy is of the form

$$G(u,u_x) = \sum_{l=1}^{M} f_l(u)g_l(u_x), \tag{13}$$

where $M \in \{1,2,\ldots\}$, and f_l, g_l are real-valued functions. For example, the local energy of the CH equation 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 $u^{(m)} \simeq u(x, m\Delta t)$, and its first derivative by $u_x^{(m)} = (\partial/\partial x)u^{(m)}$. Then the Galerkin version of the discrete variational derivative is defined as follows:

Definition 3.1 (Galerkin version of discrete variational derivative). *We call the discrete quantity*

$$\frac{\delta G_{\mathrm{d}}}{\delta(u^{(m+1)},u^{(m)})} :\equiv \frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})} - \frac{\partial}{\partial x}\left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\right) \tag{14}$$

the "(Galerkin) discrete variational derivative," where

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})} :\equiv \sum_{l=1}^{M}\left(\frac{f_l(u^{(m+1)})-f_l(u^{(m)})}{u^{(m+1)}-u^{(m)}}\right)\left(\frac{g_l(u_x^{(m+1)})+g_l(u_x^{(m)})}{2}\right), \tag{15}$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})} :\equiv \sum_{l=1}^{M}\left(\frac{f_l(u^{(m+1)})+f_l(u^{(m)})}{2}\right)\left(\frac{g_l(u_x^{(m+1)})-g_l(u_x^{(m)})}{u_x^{(m+1)}-u_x^{(m)}}\right) \tag{16}$$

are discrete partial derivatives corresponding to $\partial G/\partial u$ and $\partial G/\partial u_x$, respectively[2].

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

The following (Galerkin) discrete variation identity holds (hereafter $G(u^{(m)}, u_x^{(m)})$ is abbreviated as $G(u^{(m)})$ to save space).

Theorem 3.1 (Galerkin discrete variation identity).

$$\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x = \int_0^L \frac{\delta G_{\mathrm{d}}}{\delta(u^{(m+1)}, u^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) \mathrm{d}x + \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L. \tag{17}$$

Proof. It is straightforward to check

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

for $G(u, u_x)$ of the form given in equation (13). It is then straightforward to prove the theorem by applying integration by parts. □

For the discrete variational derivative, a dissipative Galerkin scheme is given below. Let us denote the trial space by S_{d}, and the test space by W_{d}. We also use the notation $(f, g) = \int_0^L fg\mathrm{d}x$, and $\|\cdot\|_2$ is the associated norm.

Scheme 1 (Galerkin scheme with discrete variational derivative). *Suppose that $u^{(0)}(x)$ is given in S_{d}. Find $u^{(m)} \in S_{\mathrm{d}}$ $(m = 1, 2, \ldots)$ such that, for any $v \in W_{\mathrm{d}}$,*

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v\right) = -\left(\frac{\delta G_{\mathrm{d}}}{\delta(u^{(m+1)}, u^{(m)})}, v\right). \tag{18}$$

Theorem 3.2 (Dissipation property of Scheme 1). *Assume that boundary conditions are imposed so that*

$$\left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L = 0, \tag{19}$$

and that $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{\mathrm{d}}$. 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.

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L \left(G(u^{(m+1)}) - G(u^{(m)})\right) \mathrm{d}x \\
&= \int_0^L \frac{\delta G_{\mathrm{d}}}{\delta(u^{(m+1)}, u^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) \mathrm{d}x + \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L \\
&= -\int_0^L \left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)^2 \mathrm{d}x \le 0.
\end{aligned} \tag{20}$$

Notice that in the second equality, the Galerkin scheme form (18) is used with $v = (u^{(m+1)} - u^{(m)})/\Delta t \in W_{\rm d}$. The boundary term vanishes as a result of the assumption. □

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

Thus it appears that we have succeeded in rewriting the DVDM in a Galerkin framework. However, there is a serious problem in that the scheme would require the use of expensive C^1 elements due to the discrete variational derivative $\delta G_{\rm d}/\delta(u^{(m+1)}, u^{(m)})$, which generally includes second derivatives. For example, when $G(u) = {u_x}^2/2$,

$$\frac{\delta G_{\rm d}}{\delta(u^{(m+1)}, u^{(m)})} = -\frac{u_{xx}^{(m+1)} + u_{xx}^{(m)}}{2},$$

according to definition (14). Furthermore, the situation clearly gets worse if we take into account the "additional" differentiation $(\partial/\partial x)^{2s}$ in equation (3), which leads to fourth- or higher-order derivatives that demand still smoother basis functions.

4 A Practical Galerkin discrete derivative method

Fortunately, there is an way to get around the difficulty described in the previous section. The essential ideas are that, in order to avoid the possible second derivatives in the discrete variational derivative $\delta G_{\rm d}/\delta(u^{(m+1)}, u^{(m)})$, we abandon the concept of variational derivative, and instead fully utilize partial derivatives, while, in order to cope with higher-order differentiation $(\partial/\partial x)^{2s}$, we propose to introduce appropriate intermediate variables and employ the so-called "mixed" formulation.

4.1 Real-valued PDEs (3)

The simplest case $s = 0$ and general cases $s = 1, 2, \ldots$ are treated separately.

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

$$\begin{aligned}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v\right) &= -\left(\frac{\partial G_{\rm d}}{\partial(u^{(m+1)}, u^{(m)})}, v\right) - \left(\frac{\partial G_{\rm d}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, v_x\right) \\ &\quad + \left[\frac{\partial G_{\rm d}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v\right]_0^L. \qquad (21)\end{aligned}$$

The discrete partial derivatives (15) and (16) do not include second derivatives. Thus the scheme can be implemented using only H^1 elements, such as the standard piecewise linear function space. Furthermore, curiously enough, this form is still sufficient to prove the discrete dissipation property:

Theorem 4.1 (Dissipation property of Scheme 2). *Assume that boundary conditions are imposed so that equation (19) is satisfied, and that* $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{\mathrm{d}}$. *Then Scheme 2 is dissipative in the sense that*

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

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L (G(u^{(m+1)}) - G(u^{(m)}))\,\mathrm{d}x \\
&= \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, \frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, \frac{u_x^{(m+1)} - u_x^{(m)}}{\Delta t}\right) \\
&= -\left\|\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right\|_2^2 + \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L \le 0. \qquad (22)
\end{aligned}$$

The first equality is shown in the proof of Theorem 3.1. The second one is shown by making use of expression (21) and the assumption $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{\mathrm{d}}$. The inequality is shown by the assumption regarding the boundary conditions. □

To handle the additional differentiation $(\partial/\partial x)^{2s}$, intermediate variables are introduced. Accordingly, multiple trial spaces $S_1, \ldots, S_{s+1}$, and test spaces $W_1, \ldots, W_{s+1}$, some of which can coincide, are assumed.

Scheme 3 (Galerkin scheme for $s \ge 1$). *Suppose that* $u^{(0)}(x)$ *is given in* S_{d}. *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* $v_1 \in W_1, \ldots, v_{s+1} \in W_{s+1}$,

$$\begin{aligned}
\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) &= -\left((p_1^{(m+\frac{1}{2})})_x, (v_1)_x\right) + \left[(p_1^{(m+\frac{1}{2})})_x v_1\right]_0^L, &(23)\\
\left(p_{j-1}^{(m+\frac{1}{2})}, v_j\right) &= \left((p_j^{(m+\frac{1}{2})})_x, (v_j)_x\right) - \left[(p_j^{(m+\frac{1}{2})})_x v_j\right]_0^L, &(24)\\
\left(p_s^{(m+\frac{1}{2})}, v_{s+1}\right) &= \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, v_{s+1}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_{s+1})_x\right) \\
&\quad - \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v_{s+1}\right]_0^L, &(25)
\end{aligned}$$

where in equation (24) $j = 2, 3, \ldots, s$.

Theorem 4.2 (Dissipation property of Scheme 3). *Assume that boundary conditions are imposed so that equation (19) is satisfied and* $\left[(p_{s-j+2}^{(m+\frac{1}{2})})_x \cdot p_{j-1}^{(m+\frac{1}{2})}\right]_0^L = 0$ $(j = 2, 3, \ldots, s+1)$. *Also assume that boundary conditions and the trial and test spaces are chosen such that* $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{s+1}$ *and* $S_{s-j+2} \subseteq W_{j-1}$ $(j = 2, 3, \ldots, j+1)$. *Then Scheme 3 is dissipative in the sense that*

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

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L (G(u^{(m+1)}) - G(u^{(m)}))\,\mathrm{d}x \\
&= \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)},u^{(m)})}, \frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}, \frac{u_x^{(m+1)}-u_x^{(m)}}{\Delta t}\right) \\
&= \left(p_s^{(m+\frac{1}{2})}, \frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right) - \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)},u_x^{(m)})}\left(\frac{u^{(m+1)}-u^{(m)}}{\Delta t}\right)\right]_0^L \\
&= -\left((p_1^{(m+\frac{1}{2})})_x, (p_s^{(m+\frac{1}{2})})_x\right) + \left[(p_1^{(m+\frac{1}{2})})_x p_s^{(m+\frac{1}{2})}\right]_0^L. \qquad (26)
\end{aligned}$$

The second equality is shown by using equation (25) with $v_{s+1} = (u^{(m+1)} - u^{(m)})/\Delta t$. The third equality is given by using equation (23) with $v_1 = p_s^{(m+\frac{1}{2})}$ and the assumption $S_s \subseteq W_1$. By repeatedly making use of equation (24), 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. □

Schemes 2 and 3 may appear a little unusual at first glance since the boundary terms $[\cdot]_0^L$ are included as parts of the schemes. In practice, however, these terms can be eliminated by applying the boundary conditions, and the conditions on the trial and test spaces. This may be seen in practice in the application examples in Section 5.

4.2 Complex-valued PDEs (4)

Suppose that the local energy is again of the form of equation (13), 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 $(f,g) = \int_0^L \bar{f} g \mathrm{d}x$. Complex discrete partial derivatives are defined as follows:

Definition 4.1 (complex discrete partial derivatives). *We call the discrete quantities*

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

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

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

$$\overline{\left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}\right)} = \frac{\partial G_{\mathrm{d}}}{\partial(\overline{u^{(m+1)}}, \overline{u^{(m)}})}, \quad \text{and} \quad \overline{\left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\right)} = \frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})}. \tag{29}$$

The following identity holds concerning the complex partial derivatives.

Theorem 4.3 (Complex Galerkin discrete variation identity).

$$\frac{1}{\Delta t}\int_0^L (G(u^{(m+1)}) - G(u^{(m)}))\,\mathrm{d}x = \int_0^L \frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\mathrm{d}x$$
$$+ \int_0^L \frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u_x^{(m+1)} - u_x^{(m)}}{\Delta t}\right)\mathrm{d}x + (\text{c.c.}), \tag{30}$$

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 (4) is proposed as follows:

Scheme 4 (Galerkin scheme for the PDEs (4)). *Suppose that $u^{(0)}(x)$ is given in S_{d}. Find $u^{(m)} \in S_{\mathrm{d}}$ $(m = 1, 2, \ldots)$ such that, for any $v \in W_{\mathrm{d}}$,*

$$\mathrm{i}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v\right) = -\left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u^{(m+1)}}, \overline{u^{(m)}})}, v\right) - \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})}, v_x\right)$$
$$+ \left[\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})} v\right]_0^L. \tag{31}$$

Theorem 4.4 (Conservation property of Scheme 4). *Assume that boundary conditions are imposed so that*

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

and $(u^{(m+1)} - u^{(m)})/\Delta t \in W_{\mathrm{d}}$. Then Scheme 4 is conservative in the sense that

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

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\int_0^L (G(u^{(m+1)}) - G(u^{(m)}))\,\mathrm{d}x \\
&= \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u^{(m+1)}}, \overline{u^{(m)}})}, \frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})}, \frac{u_x^{(m+1)} - u_x^{(m)}}{\Delta t}\right) + (\text{c.c.}) \\
&= -\mathrm{i}\left\|\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right\|_2^2 + \left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}\right)\right]_0^L + (\text{c.c.}) \\
&= 0.
\end{aligned} \tag{32}$$

□

5 Application examples

Examples of the application of the proposed method are described in this section. Due to the restriction of space, we only show that two prominent dissipative/conservative Galerkin schemes in the literature can be derived from, i.e. regarded as examples of, the proposed method. 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.

5.1 The Cahn-Hilliard equation

The CH equation (1) is an example of equation (3) with $s = 1$ and $G(u, u_x) = pu^2/2 + ru^4/4 - qu_x^2/2$, which is usually solved subject to the boundary conditions

$$u_x = 0 \quad \text{and} \quad \frac{\partial}{\partial x}\left(\frac{\delta G}{\delta u}\right) = 0 \qquad \text{at } x = 0, L. \tag{33}$$

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 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 $v_2 \in W_2$,

$$\left(\frac{u^{(m+1)} - u^{(m)}}{\Delta t}, v_1\right) = -\left((p_1^{(m+\frac{1}{2})})_x, (v_1)_x\right), \tag{34}$$

$$\left(p_1^{(m+\frac{1}{2})}, v_2\right) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})}, v_2\right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})}, (v_2)_x\right) \tag{35}$$

hold, where the terms

$$\begin{aligned} \frac{\partial G_{\mathrm{d}}}{\partial(u^{(m+1)}, u^{(m)})} &= p\left(\frac{u^{(m+1)} + u^{(m)}}{2}\right) + \\ &\quad r\left(\frac{(u^{(m+1)})^2 + (u^{(m)})^2}{2}\right)\left(\frac{u^{(m+1)} + u^{(m)}}{2}\right), \end{aligned} \tag{36}$$

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

are obtained from definitions (15) and (16). Note that the boundary term $\left[(p_1^{(m+\frac{1}{2})})_x v_1\right]_0^L$ which should appear in equation (34) and also the $\left[\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(m+1)}, u_x^{(m)})} v_2\right]_0^L$ term in (35) 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 4.2 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 zero Dirichlet boundary conditions.

Remark 5.1. 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 (33) are automatically recovered as the natural boundary conditions.

5.2 The nonliear Schrödinger equation

Let us consider the NLS equation (2) under the periodic boundary conditions:

$$u(0,t) = u(L,t), \quad \text{and} \quad u_x(0,t) = u_x(L,t), \qquad t > 0. \tag{38}$$

This is an example of equation (4) with $G(u,u_x) = -|u_x|^2 + 2\gamma|u|^{p+1}/(p+1)$. Let us select the trial and test spaces $S_\mathrm{d} = W_\mathrm{d} = \{v \mid v \in S_h,\ v(0) = v(L)\}$. Then Scheme 4 becomes: find $u \in S_\mathrm{d}$ such that, for all $v \in W_\mathrm{d}$,

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

where the terms

$$\frac{\partial G_\mathrm{d}}{\partial(\overline{u^{(m+1)}}, \overline{u^{(m)}})} = \gamma\left(\frac{|u^{(m+1)}|^{p+1} - |u^{(m)}|^{p+1}}{|u^{(m+1)}|^2 - |u^{(m)}|^2}\right)\left(\frac{u^{(m+1)} + u^{(m)}}{2}\right), \tag{39}$$

$$\frac{\partial G_\mathrm{d}}{\partial(\overline{u_x^{(m+1)}}, \overline{u_x^{(m)}})} = -\frac{u_x^{(m+1)} + u_x^{(m)}}{2}, \tag{40}$$

are obtained from definitions (27) and (28). The boundary term appearing in equation (31) vanishes due to the periodicity of S_d and W_d. The periodicity also implies that condition (19) is satisfied, and thus the conservation property follows from Theorem 4.4. It may be noted that this scheme is simply the Akrivis-Dougalis-Karakashian scheme [1].

6 Concluding remarks

In this paper a new method for the automatic design of dissipative/conservative Galerkin schemes is proposed. It is then shown that two novel schemes in the literature can be regarded as special cases of the present method.

Finally, we would like to emphasize the following issues, which could not have been covered in this article due to the restriction of space.

- **New schemes by the present method:** Several new dissipative/conservative Galerkin schemes can be derived by the present method. For example, a new conservative Galerkin scheme for the Korteweg-de Vries equation has been discovered [10]. We are now investigating the scheme both experimentally and theoretically.

- **Extension to two- or three-dimensional cases:** The essential idea is also valid in two- or three-dimensional cases, whereas more careful considerations on boundary and spatial integrations are required in such circumstances.

These issues will be discussed elsewhere in the near future.

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References

[1] G. D. Akrivis, V. A. Dougalis and O. A. Karakashian, On fully discrete Galerkin methods of second-order temporal accuracy for the nonlinear Schrödinger equation, *Numer. Math.*, **59** (1991), 31–53.

[2] G. Ben-Yu, P. J. Pascual, M. J. Rodriguez and L. Vázquez, Numerical solution of the sine-Gordon equation, *Appl. Math. Comput.*, **18** (1986), 1–14.

[3] C. J. Budd and M. D. Piggott, Geometric integration and its applications, *Handbook of numerical analysis*, **XI**, North-Holland, Amsterdam, 2003, 35–139.

[4] Q. Du and R. A. Nicolaides, Numerical analysis of a continuum model of phase transition, *SIAM J. Numer. Anal.*, **28** (1991), 1310–1322.

[5] D. Furihata, 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, *J. Comput. Phys.*, **156** (1999), 181–205.

[6] S. Li and L. Vu-Quoc, Finite difference calculus invariant structure of a class of algorithms for the nonlinear Klein-Gordon equation, *SIAM J. Numer. Anal.*, **32** (1995), 1839–1875.

[7] T. Matsuo, Discrete variational method and its various extensions, Ph.D. Thesis, Department of Engineering, University of Tokyo, 2003.

[8] T. Matsuo, A conservative Galerkin scheme for the KdV equation, Book of Abstracts of the First China-Japan-Korea Joint Conference on Numerical Mathematics (Hokkaido University Technical Report Series in Mathematics No. 112), 2006, 41–42. (`http://www.sr3.t.u-tokyo.ac.jp/~matsuo/preprints/cjk.pdf`)

[9] T. Matsuo and D. Furihata, Dissipative or conservative finite difference schemes for complex-valued nonlinear partial differential equations, *J. Comput. Phys.* **171** (2001), 425–447.

[10] T. Matsuo, M. Sugihara, D. Furihata and M. Mori, Spatially accurate dissipative or conservative finite difference schemes derived by the discrete variational method, *Japan J. Indust. Appl. Math.*, **20** (2003), 311-330.

[11] W. Strauss and L. Vazquez, Numerical solution of a nonlinear Klein-Gordon equation, *J. Comput. Phys.*, **28** (1978), 271–278.