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A Novel Semi-Analytical Multiple Invariants-Preserving Integrator for Conservative PDEs

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Abstract. Many conservative partial differential equations such as the Korteweg-de Vries (KdV) equation, the nonlinear Schrödinger equation, and the Klein-Gordon equation have more than one invariant functionals. In this paper, we propose the definition of the discrete variational derivative, based on which, a novel semi-analytical multiple invariants-preserving integrator for the conservative partial differential equations is constructed by projection technique. The proposed integrators, constructed by applying a projection technique to existing numerical methods, are shown to preserve the same order of accuracy as their underlying base integrators. For applications, some concrete mass-momentum-energy-preserving integrators are derived for the KdV equation.

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Key words: Conservative partial differential equation, invariants-preserving, discrete variational derivative, projection, Korteweg-de Vries equation.

1. Introduction

It is known that partial differential equation (PDE) plays an important role in science and engineering. It can describe many phenomena in physics, engineering, chemistry, and other sciences. Much attention has been paid to investigating the analytical solutions of partial differential equations [17, 22, 28, 44]. The investigation on analytical solutions can offer the physicists and engineers a powerful tool to examine the

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feasibility of the model by adjusting some physical parameters, and give good enough support to numerical simulation. However, generally speaking, the analytical solutions of PDEs are not available. Hence, the development of numerical integrators for PDEs is required.

Many PDEs such as the KdV equation, and the nonlinear Schrödinger equations, the Klein-Gordon equation can be expressed in nonlinear Hamiltonian form. An important feature of Hamiltonian systems is that they admit conservation law structures which are fundamental to the derivation of analytical solutions, the analysis of the qualitative behaviours, and the numerical discretization of the systems. It has become common practice that numerical integrators should be designed to retain the conservation law structures or other geometric structures, which will be more preferable when studying the long-time behaviour of dynamical systems. Such numerical integrators are usually called geometric or structure-preserving. We refer the reader to [19, 27, 30, 35, 40, 41] for recent surveys of this research. In this paper, we focus ourselves on the energy/invariants-preserving integrator, which is a typical branch of structure-preserving integrators. For ordinary differential equations (ODEs), a variety of invariant-preserving integrators, such as the continuous-stage Runge-Kutta (-Nyström) (RK(N)) integrators [26], the discrete gradient integrators [10, 13, 15, 37], the Hamiltonian boundary value methods [6–8], have been developed in relatively general frameworks. In comparison, the construction of the invariant-preserving integrators for PDEs seems more complicated since PDEs are a huge and motley collection of problems and a case-by-case discussion is required to devise the invariant-preserving integrators for each partial differential equation under consideration (see, e.g. [9–11]). Some progress has been made to give a fairly general framework to develop invariant-preserving integrators for PDEs. In [10], by using the method of lines and the average vector field method, a systematic procedure to construct invariant-preserving schemes for evolutionary PDEs is developed. By reformulating the PDEs into multi-symplectic Hamiltonian forms, many energy-preserving or multi-symplectic methods are derived (see, e.g., [3, 12, 24, 29]). Furihata [20, 21], Matsuo and Furihata [34] presented the concept of discrete variational derivatives, based on which, finite-difference schemes that inherit energy conservation property are derived for PDEs. In [15], a general procedure for constructing linearly implicit conservative numerical integrators for PDEs is presented. All the procedures mentioned above require the semidiscretization of the PDEs in space.

In this paper, we consider invariant-preserving integrators for PDEs in a semi-analytical framework. To be more precise, we focus on time-stepping numerical integrators and do not require the PDEs to be discretized in spatial direction. The benefit is that it does not depend on the number of independent variables and the order of derivatives in space. Therefore, it is applicable to a wider range of PDE models. We firstly extend the concept of discrete gradient for gradient of a function to the variational derivative of a functional. Then, a semi-analytical discrete variational derivative integrator will be derived for the conservative PDEs. The variational derivative integrator preserves the energy exactly. Furthermore, multiple invariants-preserving integrators for conservative PDEs that have more than one conservation laws will also be constructed by using projection.

The outline of this paper is as follows. Some preliminaries are presented and the definition of the discrete variational derivative is proposed in Section 2. In Section 3, the novel semi-analytical energy-preserving integrators and the multiple invariants-preserving integrators are constructed based on the discrete variational derivative and projection. Some properties of the proposed integrators are discussed as well. For applications, some concrete invariants-preserving integrators are constructed for the KdV equation in Section 4. The last section focuses on some conclusions and discussions.

2. Preliminaries and the discrete variational derivative

We consider nonlinear first-order conservative PDE with the Hamiltonian formulation

$$\begin{cases} \dfrac{\partial u}{\partial t} = \mathcal{J}\dfrac{\delta \mathcal{G}}{\delta u}, \\ u(t_0) = u_0, \end{cases} \tag{2.1}$$

where $\mathcal{J}$ is a skew adjoint operator, the energy functional

$$\mathcal{G}[u] = \int_\Omega G[u]dx, \quad \Omega \subseteq \mathbb{R}^d, \tag{2.2}$$

and $u : \mathbb{R}^d \times [t_0, +\infty] \to \mathbb{R}$, $dx = dx_1 \cdots dx_d$. We use the square brackets in (2.2) to indicate that the energy functional $\mathcal{G}$ and the local energy density G depend on the function u as well as derivatives of u with respect to the independent variables $x = (x_1, \cdots, x_d)$ up to some degree ν. The variational derivative $\delta\mathcal{G}/\delta u$ is defined by the relation

$$\int_\Omega \frac{\delta \mathcal{G}}{\delta u} v dx = \frac{d}{d\epsilon}\Big|_{\epsilon=0} \mathcal{G}[u + \epsilon v] \tag{2.3}$$

for any sufficiently smooth function $v(x)$. Here and from now on, the solution of (2.1) is assumed to have sufficient regularity and the equipped boundary conditions on Ω of (2.1) satisfies that the boundary terms vanish when calculating integration by parts (for example, periodic boundary conditions, zero Dirichlet boundary conditions).

For the case of $d = 1$, suppose

$$\mathcal{G}[u] = \int_\Omega G\left(u, \frac{\partial u}{\partial x}, \ldots, \frac{\partial^k u}{\partial x^k}\right) dx.$$

Then it can be derived that

$$\frac{\delta \mathcal{G}}{\delta u} = \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\left(\frac{\partial G}{\partial u_x}\right) + \frac{\partial}{\partial x^2}\left(\frac{\partial G}{\partial u_{xx}}\right) + \cdots + (-1)^k \frac{\partial}{\partial x^k}\left(\frac{\partial G}{\partial u^{(k)}}\right).$$

For the case of $d \geqslant 2$, one can apply the Euler operator to $G[u]$ to obtain the variational derivatives (see e.g. [15] for details).

Denote $\mathcal{F}(\Omega) \subset L^2(\Omega)$ as the function space that the solution $u(\cdot,t)$ lies in. By our assumption, the equation of the form (2.1) has in common the energy conservation property

$$\frac{d}{dt}\mathcal{G}[u] = 0. \tag{2.4}$$

The key idea to construct energy-preserving integrators for (2.1) is to introduce the concept of discrete variational derivative (DVD).

Definition 2.1. *The function $\delta\mathcal{G}/\delta(u,v) \in L^2(\Omega)$ is a discrete variational derivative of the functional $\mathcal{G}$ provided that for any functions $u, v \in \mathcal{F}(\Omega)$, $u \neq v$, satisfying*

$$\begin{cases} \mathcal{G}[u] - \mathcal{G}[v] = \displaystyle\int_\Omega \frac{\delta\mathcal{G}}{\delta(u,v)} \cdot (u-v)\mathrm{d}x := \left\langle \frac{\delta\mathcal{G}}{\delta(u,v)}, u-v \right\rangle, \\ \dfrac{\delta\mathcal{G}}{\delta(u,u)} = \dfrac{\delta\mathcal{G}}{\delta u}, \end{cases} \tag{2.5}$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product of $L^2(\Omega)$

$$\langle v, w\rangle = \int_\Omega vw dx.$$

The discrete variational derivative can be regarded as a continuous generalization of discrete gradient for the gradient of a function. The concept of discrete gradient leads to the discrete gradient methods for ordinary differential equations. We refer the reader to [13, 25, 31, 36–39] for more research on this topic.

The simplest discrete variational derivative of $\mathcal{G}$ is

$$\frac{\delta\mathcal{G}}{\delta(u,v)} = \frac{G[u]-G[v]}{u-v}. \tag{2.6}$$

Similar argument as the average vector field (AVF), one of the frequently used discrete gradients, yields the AVF-type discrete variational derivative

$$\frac{\delta\mathcal{G}_{\mathrm{AVF}}}{\delta(u,v)} = \int_0^1 \frac{\delta\mathcal{G}}{\delta u}[\xi u + (1-\xi)v]\mathrm{d}\xi. \tag{2.7}$$

As a matter of fact, we can verify that

$$\begin{aligned} \mathcal{G}[u] - \mathcal{G}[v] &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\xi}\mathcal{G}[\xi u + (1-\xi)v]\mathrm{d}\xi \\ &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0}\mathcal{G}[v + (\xi+\varepsilon)(u-v)]\mathrm{d}\xi \\ &= \int_0^1 \int_\Omega \frac{\delta\mathcal{G}}{\delta u}[\xi u + (1-\xi)v]\cdot(u-v)\mathrm{d}x\mathrm{d}\xi \\ &= \int_\Omega \int_0^1 \frac{\delta\mathcal{G}}{\delta u}[\xi u + (1-\xi)v]\mathrm{d}\xi \cdot (u-v)\mathrm{d}x. \end{aligned}$$

Therefore, (2.7) is indeed a discrete variational derivative of $\mathcal{G}[u]$.

Remark 2.1. The concept of discrete variational derivative is different from the "discrete variational derivative" given in [20]. It has appeared in [15] but has not been discussed under the analytical framework in details.

Remark 2.2. Given the generality of our framework, we are unable to provide specific assumptions to guarantee that the discrete variational derivatives defined by (2.6) and (2.7) will lie in $L^2(\Omega)$ for arbitrary energy functionals. However, for the specific classes of problems and energy functionals considered in this work (particularly those arising in our numerical examples), these discrete variational derivatives do belong to $L^2(\Omega)$.

3. The semi-analytical discrete variational derivative integrator for (2.1)

Based on the discrete variational derivatives, we can construct the semi-analytical discrete variational derivative integrator for (2.1). The semi-analytical DVD integrator takes the form

$$\frac{u^{k+1}(x)-u^k(x)}{\Delta t}=\mathcal{J}\frac{\delta\mathcal{G}}{\delta(u^{k+1}(x),u^k(x))},\quad k=0,1,\dots, \tag{3.1}$$

where $u^k(x)$ is an approximation to the exact solution $u(x,t_k)$ at $t_k=t_0+k\Delta t$ which is obtained by k steps of the semi-analytical DVD integrator. Using discrete variational derivatives (2.6) and (2.7) yields two concrete semi-analytical DVD integrators

$$\frac{u^{k+1}(x)-u^k(x)}{\Delta t}=\mathcal{J}\frac{G[u^{k+1}(x)]-G[u^k(x)]}{u^{k+1}(x)-u^k(x)},\qquad k=0,1,\dots, \tag{3.2}$$

$$\frac{u^{k+1}(x)-u^k(x)}{\Delta t}=\mathcal{J}\int_0^1\frac{\delta\mathcal{G}}{\delta u}\Big[\xi u^{k+1}(x)+(1-\xi)u^k(x)\Big]\,\mathrm{d}\xi,\quad k=0,1,\dots. \tag{3.3}$$

Remark 3.1. Here, for simplicity, we assume that the skew adjoint operator $\mathcal{J}$ is independent of the function u. Otherwise, the discretization of the skew adjoint operator $\mathcal{J}[u]$ can be taken as $\mathcal{J}[(u^{k+1}(x)+u^k(x))/2]$ in the semi-analytical discrete variational derivative integrator (3.1).

Typically speaking, the conservative PDE (2.1) may have more than one conserved functionals. Correspondingly, the PDE (2.1) has more than one Hamiltonian formulations. We may apply the semi-analytical DVD integrator to the particular Hamiltonian formulation corresponding to the functional to be preserved. Unfortunately, the semi-analytical DVD integrator (3.1) cannot preserve more than one conserved functionals at the same time in general. We will address this issue in what follows. Assume that the Eq. (2.1) possesses n independent invariant functionals

$$\mathcal{H}_1[u]=\int_\Omega H_1[u]dx,\quad \mathcal{H}_2[u]=\int_\Omega H_2[u]dx,\cdots,\mathcal{H}_n[u]=\int_\Omega H_n[u]dx. \tag{3.4}$$

Our target is to construct a semi-analytical integrator that can preserve all the invariants (3.4). Due to the conservation of the invariants (3.4), the solution of system (2.1) lies on the submanifold

$$M = \big\{u \in \mathcal{F}(\Omega) : \mathcal{H}_1(u) = \mathcal{H}_1(u_0), \mathcal{H}_2(u) = \mathcal{H}_2(u_0), \cdots, \mathcal{H}_n(u) = \mathcal{H}_n(u_0)\big\}.$$

The tangent space T_uM ([15]) of M at u is the orthogonal complement space to the linear space

$$\text{span}\left\{\frac{\delta\mathcal{H}_1}{\delta u}, \frac{\delta\mathcal{H}_2}{\delta u}, \cdots, \frac{\delta\mathcal{H}_n}{\delta u}\right\} \subset L^2(\Omega),$$

where the orthogonality is in the sense of the inner product of $L^2(\Omega)$.

Definition 3.1. *Let $\delta\mathcal{H}/\delta(u,v)$ be a fixed discrete variational derivative of $\mathcal{H}[u]$. The discrete tangent space at $(v,w) \in \mathcal{F}(\Omega)\times\mathcal{F}(\Omega)$ is*

$$T_{(v,w)}M = \left\{\eta \in \mathcal{F}(\Omega) : \left\langle \frac{\delta\mathcal{H}_1}{\delta(v,w)}, \eta\right\rangle = \left\langle \frac{\delta\mathcal{H}_2}{\delta(v,w)}, \eta\right\rangle = \cdots = \left\langle \frac{\delta\mathcal{H}_n}{\delta(v,w)}, \eta\right\rangle = 0\right\}.$$

A vector $\eta = \eta_{(v,w)} \in T_{(v,w)}M$ is called a discrete tangent vector.

The following lemma plays an important role in deriving the multiple invariants-preserving integrators. The statement and the proof are similar to that of [15, Lemma 2.2].

Lemma 3.1. *Let $u^{k+1}(x) = \varphi_h(u^k(x))$ be a semi-analytical time-stepping integrator for the Eq.* (2.1). *It preserves the n invariants* (3.4) *simultaneously in the sense that*

$$\begin{aligned}
&\mathcal{H}_1\big(u^{k+1}(x)\big) = \mathcal{H}_1\big(u^k(x)\big), \quad \mathcal{H}_2\big(u^{k+1}(x)\big) = \mathcal{H}_2(u^k(x)), \cdots, \\
&\mathcal{H}_n\big(u^{k+1}(x)\big) = \mathcal{H}_n\big(u^k(x)\big) \quad k = 0,1,2,\ldots,
\end{aligned}$$

providing that

$$\eta_{(u^{k+1}(x),u^k(x))} := \frac{u^{k+1}(x) - u^k(x)}{\Delta t} \in T_{(u^{k+1}(x),u^k(x))}M.$$

Proof. Since $\eta_{(u^{k+1},u^k)} \in T_{(u^{k+1},u^k)}M$, it can be verified that

$$\begin{aligned}
&\mathcal{H}_i\big(u^{k+1}(x)\big) - \mathcal{H}_i\big(u^k(x)\big) \\
&= \int_\Omega \frac{\delta\mathcal{H}_i}{\delta(u^{k+1}(x), u^k(x))}\cdot\big(u^{k+1}(x) - u^k(x)\big)dx \\
&= \Delta t\left\langle \frac{\delta\mathcal{H}_i}{\delta(u^{k+1}(x), u^k(x))}, \eta_{(u^{k+1}(x),u^k(x))}\right\rangle = 0, \quad k = 0,1,2,\ldots, \quad i = 1,2,\ldots,n.
\end{aligned}$$

The proof is complete. □

In what follows, we present a general framework to construct the multiple invariants-preserving integrator by using the projection technique. Let

$$\begin{aligned}
&Y\big(u^{k+1}(x), u^k(x)\big) \\
&= \text{span}\left\{\frac{\delta\mathcal{H}_1}{\delta(u^{k+1}(x),u^k(x))}, \frac{\delta\mathcal{H}_2}{\delta(u^{k+1}(x),u^k(x))}, \cdots, \frac{\delta\mathcal{H}_n}{\delta(u^{k+1}(x),u^k(x))}\right\}
\end{aligned}$$

be the subspace spanned by the discrete variational derivatives of $\mathcal{H}_i[u], i = 1, 2, \ldots, n$ at $(u^{k+1}(x), u^k(x))$. Assume that $\{w^1(x), w^2(x), \cdots, w^n(x)\}$ is an orthogonal basis of $Y(u^{k+1}(x), u^k(x))$ which can be obtained by the classical Gram-Schmidt procedure. Then the projection operator

$$\mathcal{P}\big(u^{k+1}(x), u^k(x)\big)v(x) = v(x) - \sum_{i=1}^{n} \big\langle v(x), w^i(x)\big\rangle\, w^i(x)$$

would be a smooth orthogonal projection operator onto the discrete tangent space $T_{(u^{k+1}(x), u^k(x))}M$. We propose the projection integrator

$$u^{k+1}(x) = u^k(x) + \mathcal{P}\big(u^{k+1}(x), u^k(x)\big)\big(\psi_h(u^k(x)) - u^k(x)\big), \tag{3.5}$$

or equivalently

$$y^{k+1}(x) = \psi_h\big(u^k(x)\big), \quad u^{k+1}(x) = u^k(x) + \mathcal{P}\big(u^{k+1}(x), u^k(x)\big)\big(y^{k+1}(x) - u^k(x)\big), \tag{3.6}$$

where ψ_h is the flow that defines an arbitrary integrator of order p. It is easy to see that the projection integrator (3.6) satisfies the condition in Lemma 3.1. Hence, it preserves the n invariants (3.4).

Remark 3.2. The operator $\mathcal{I} - \mathcal{P}(u^{k+1}(x), u^k(x))$ is nothing but the orthogonal projection operator onto the space $Y(u^{k+1}(x), u^k(x))$.

Remark 3.3. If both the discrete variational derivatives $\delta\mathcal{H}_i/\delta(u^{k+1}, u^k), i = 1, 2, \ldots, n$ and the underlying integrator ψ_h are symmetric, then the integrator (3.6) is symmetric as well.

Using Runge-Kutta (RK) integrator as the underlying integrator ψ_h, we can construct concrete multiple invariants-preserving integrators.

Definition 3.2. *An s-stage RK integrator for the Eq.* (2.1) *reads*

$$\begin{cases} U^{k,i}(x) = u^k(x) + \Delta t \displaystyle\sum_{j=1}^{s} a_{ij} f\big(U^{k,j}(x)\big), & i = 1, \ldots, s, \\ u^{k+1}(x) = u^k(x) + \Delta t \displaystyle\sum_{i=1}^{s} b_i f\big(U^{k,i}(x)\big), & k = 0, 1, \ldots, \end{cases} \tag{3.7}$$

where $a_{ij}, b_i, c_i, i, j = 1, \ldots, s$ are real constants, $f(u) = \mathcal{J}(\delta\mathcal{G}/\delta u)$, $u^k(x)$ denotes the numerical solution after k steps of the integrator and is an approximation to the exact solution $u(x, t_k)$, while the internal stage value $U^{k,i}(x)$ is an approximation to $u(x, t_k + c_i\Delta t)$.

The RK integrator (3.7) can be briefly expressed by the following Butcher tableau:

$$\begin{array}{c|c} c & A \\ \hline & b^\top \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array},$$

where $b=(b_1,\dots,b_s)^\top$ and $c=(c_1,\dots,c_s)^\top$ are s-dimensional vectors, and $A=(a_{ij})$ is an $s\times s$ matrix. If $a_{ij}=0$ for all $1\le i\le j\le s$, the integrator (3.7) is explicit, otherwise it is implicit.

Definition 3.3. *The projection RK integrator for the Eq.* (2.1) *reads*

$$\begin{cases} U^{k,i}(x)=u^k(x)+h\sum_{j=1}^{s}a_{ij}f\big(U^{k,j}(x)\big), & i=1,\dots,s,\\ u^{k+1}(x)=u^k(x)+h\mathcal{P}\left(u^{k+1}(x),u^k(x)\right)\sum_{i=1}^{s}b_if\big(U^{k,i}(x)\big), & k=0,1,\dots. \end{cases} \tag{3.8}$$

It should be noted that regardless of whether the underlying RK method is explicit or implicit, the corresponding projection RK integrator will be implicit since $u^{k+1}(x)$ appears in the projection operator. This implicit nature may relax the Courant-Friedrichs-Lewy (CFL) condition compared to the original explicit method. Meanwhile, the implementation considerations remain essentially the same for any choice of underlying method.

Our approach primarily leverages the algebraic accuracy rather that other properties of the base integrator. Certain desirable properties of the underlying integrator may be inevitably altered by the projection process. Despite that, the underlying integrator gains enhanced properties, particularly the conservation of multiple invariants, through projection process. This trade-off is fundamental to our methodology, as it enables the construction of high-order algorithms with improved structure-preserving capabilities.

Remark 3.4. Since the projection integrator defined above is implicit due to the dependence of the projector on u^{k+1}, the nonlinear system must be solved iteratively at each time step. In practice, both fixed-point iteration and Newton-type methods have proven effective for this purpose. While this introduces additional computational cost compared to explicit methods, it enables exact conservation of multiple invariants. We note that this implicit character is shared by most invariant-preserving integrators in the literature, making our approach consistent with established practices in this field. For problems with special structure, more efficient implementations may be possible, though such considerations are beyond the scope of this paper.

Theorem 3.1. *If the underlying integrator is of order p, then the projection integrator* (3.6) *is of order p as well, i.e.,*

$$\|u(x,t+h)-u(x,t)-\mathcal{P}(u(x,t+h),u(x,t))\left(\psi_h(u(x,t))-u(x,t)\right)\|=\mathcal{O}\left(h^{p+1}\right).$$

Proof. Let $\{w^1(x),w^2(x),\cdots,w^n(x)\}$ be an orthogonal basis of

$$\begin{aligned} &Y\big(u(x,t+h),u(x,t)\big)\\ &=\operatorname{span}\left\{\frac{\delta\mathcal{H}_1}{\delta(u(x,t+h),u(x,t))},\frac{\delta\mathcal{H}_2}{\delta(u(x,t+h),u(x,t))},\cdots,\frac{\delta\mathcal{H}_n}{\delta(u(x,t+h),u(x,t))}\right\}, \end{aligned}$$

then

$$\mathcal{P}\big(u(x,t+h),u(x,t)\big)v(x)=v(x)-\sum_{i=1}^{n}\big\langle v(x),w^i(x)\big\rangle\, w^i(x).$$

We compute

$$\begin{aligned}
&\|u(x,t+h)-u(x,t)-\mathcal{P}(u(x,t+h),u(x,t))\,(\psi_h(u(x,t))-u(x,t))\|\\
=&\Bigg\|u(x,t+h)-u(x,t)-(\psi_h(u(x,t))-u(x,t))\\
&\quad-\sum_{i=1}^{n}\big\langle \psi_h(u(x,t))-u(x,t),w^i(x)\big\rangle\, w^i(x)\Bigg\|\\
\leqslant&\ \|u(x,t+h)-u(x,t)-(\psi_h(u(x,t))-u(x,t))\|\\
&\quad+\Bigg\|\sum_{i=1}^{n}\big\langle \psi_h(u(x,t))-u(x,t),w^i(x)\big\rangle\, w^i(x)\Bigg\|\\
=&\ \|u(x,t+h)-\psi_h(u(x,t))\|+\sqrt{\sum_{i=1}^{n}\langle \psi_h(u(x,t))-u(x,t),w^i(x)\rangle^2}.
\end{aligned}\tag{3.9}$$

Since ψ_h is of order p, we have

$$\|u(x,t+h)-\psi_h(u(x,t))\|=\mathcal{O}\left(h^{p+1}\right).\tag{3.10}$$

In the following, we give the estimate of $\langle\psi_h(u(x,t))-u(x,t),w^i(x)\rangle,\ i=1,2,\ldots,n.$ Bearing in mind that both $\{w^1(x),w^2(x),\cdots,w^n(x)\}$ and

$$\left\{\frac{\delta\mathcal{H}_1}{\delta(u(x,t+h),u(x,t))},\frac{\delta\mathcal{H}_2}{\delta(u(x,t+h),u(x,t))},\cdots,\frac{\delta\mathcal{H}_n}{\delta(u(x,t+h),u(x,t))}\right\}$$

are bases of $Y(u(x,t+h),u(x,t))$, there exist some real constants d_{ij} such that

$$w^i(x)=\sum_{j=1}^{n}d_{ij}\frac{\delta\mathcal{H}_j}{\delta(u(x,t+h),u(x,t))},\quad i=1,2,\ldots,n.$$

Hence,

$$\begin{aligned}
&\big\langle\psi_h(u(x,t))-u(x,t),w^i(x)\big\rangle\\
=&\left\langle\psi_h(u(x,t))-u(x,t+h)+u(x,t+h)-u(x,t),\sum_{j=1}^{n}d_{ij}\frac{\delta\mathcal{H}_j}{\delta(u(x,t+h),u(x,t))}\right\rangle\\
=&\underbrace{\sum_{j=1}^{n}d_{ij}\left\langle\psi_h(u(x,t))-u(x,t+h),\frac{\delta\mathcal{H}_j}{\delta(u(x,t+h),u(x,t))}\right\rangle}_{\mathcal{O}(h^{p+1})}
\end{aligned}$$

$$+\underbrace{\sum_{j=1}^{n} d_{ij} \left\langle u(x,t+h)-u(x,t), \frac{\delta \mathcal{H}_j}{\delta(u(x,t+h),u(x,t))} \right\rangle}_{0}. \tag{3.11}$$

Here, the first term of the final expression in Eq. (3.11) is of order $\mathcal{O}(h^{p+1})$, which follows from Eq. (3.10). The second term vanishes due to the definition of the discrete variational derivative. Therefore,

$$\left\langle \psi_h(u(x,t)) - u(x,t), w^i(x) \right\rangle = \mathcal{O}(h^{p+1}), \quad i = 1,2,\ldots,n. \tag{3.12}$$

The proof is completed by combining the results of (3.9), (3.10) and (3.12). □

Remark 3.5. The discussion of numerical stability is of paramount importance for the numerical integrators, and it is well recognized that numerical methods may exhibit order reduction under certain circumstances when applied to PDEs. However, due to the highly general nature of our framework, we cannot provide unified results concerning stability and order reduction that would apply to all possible PDEs and spatial discretizations. The primary contribution of our work is to provide a general framework for constructing numerical integrators that preserve multiple invariants for PDEs. We note that while invariants preservation often help improve numerical stability of traditional methods, detailed numerical stability and order reduction analysis remain problem-dependent. These issues typically require case-by-case analysis that depends on the specific PDE, spatial discretization method, and boundary conditions employed. Such detailed investigations are beyond the scope of this paper.

4. Application to the KdV equation

Various aspects of the Korteweg-de Vries equation have been studied extensively in the literature [23,32,33,42]. Here, as an example of application to conservative partial differential equations, we consider the KdV equation of the classical form [1]

$$u_t(x,t) = \alpha u(x,t)u_x(x,t) + \nu u_{xxx}(x,t), \quad (x,t) \in [-l,l] \times [0,T] \tag{4.1}$$

with periodic boundary condition

$$u(-l,t) = u(l,t), \quad t \in [0,T] \tag{4.2}$$

and initial condition

$$u(x,0) = u_0(x), \quad x \in [-l,l], \tag{4.3}$$

where α, ν are real constants. The KdV equation has a great number of applications in various branches of physical science such as fluid dynamics, aerodynamics, and continuum mechanics [14,16,18,43].

4.1. Temporal semi-analytical discretization

The KdV equation (4.1) can be presented in the Hamiltonian form

$$\begin{cases} u_t = \mathcal{J}\dfrac{\delta \mathcal{G}}{\delta u}, & (x,t) \in [-l,l] \times [0,T], \\ u(-l,t) = u(l,t), & t \in [0,T], \\ u(x,0) = \psi(x), & x \in [-l,l], \end{cases} \tag{4.4}$$

where the skew adjoint operator $\mathcal{J} = \partial_x$ and the Hamiltonian

$$\mathcal{G}[u] = \int_{-l}^{l} \left(\frac{\alpha}{6} u^3 - \frac{\nu}{2} u_x^2 \right) dx =: \int_{-l}^{l} G(u, u_x) dx. \tag{4.5}$$

The variational derivative of $\mathcal{G}[u]$ can be computed as

$$\frac{\delta \mathcal{G}}{\delta u} = \frac{\partial G}{\partial u} - \partial_x \left(\frac{\partial G}{\partial u_x} \right) = \frac{\alpha}{2} u^2 + \nu u_{xx}.$$

The two semi-analytical DVD integrators proposed in the paper for the KdV equation (4.1) are

$$\begin{aligned} \frac{u^{k+1}(x) - u^k(x)}{h} &= \partial_x \Bigg(\frac{\alpha}{6} ((u^{k+1}(x))^2 + u^{k+1}(x) u^k(x) + (u^k(x))^2) \\ &\qquad - \frac{\nu}{2} \frac{(u_x^{k+1}(x))^2 - (u_x^k(x))^2}{u^{k+1}(x) - u^k(x)} \Bigg), \quad k = 0, 1, \ldots, \end{aligned} \tag{4.6}$$

$$\begin{aligned} \frac{u^{k+1}(x) - u^k(x)}{h} &= \partial_x \left(\frac{\alpha}{6} ((u^{k+1}(x))^2 + u^{k+1}(x) u^k(x) + (u^k(x))^2) \right) \\ &\qquad + \frac{\nu}{2} \big(u_{xxx}^{k+1}(x) + u_{xxx}^k(x) \big), \quad k = 0, 1, \ldots. \end{aligned} \tag{4.7}$$

The KdV equation (4.1), as a completely integrable system, actually has infinite number of invariants. Here, we are concerned with the following three invariant functionals:

- Mass:
$$\mathcal{H}_1[u] = \int_{-l}^{l} u dx. \tag{4.8}$$

- Momentum:
$$\mathcal{H}_2[u] = \frac{1}{2} \int_{-l}^{l} u^2 dx. \tag{4.9}$$

- Energy:
$$\mathcal{H}_3[u] = \int_{-l}^{l} \left(\frac{\alpha}{6} u^3 - \frac{\nu}{2} u_x^2 \right) dx. \tag{4.10}$$

The variational derivatives of $\mathcal{H}_i[u],\ i=1,2,3$ can be easily derived as

$$\frac{\delta\mathcal{H}_1}{\delta u}=1,\quad \frac{\delta\mathcal{H}_2}{\delta u}=u,\quad \frac{\delta\mathcal{H}_3}{\delta u}=\frac{\alpha}{2}u^2+\nu u_{xx}.$$

Now, we present a concrete projection RK integrator for the KdV equation (4.1). Here, the AVF-type discrete variational derivative (2.7) is chosen as the discrete variational derivative. Then the projection RK integrator reads

$$u^{k+1}(x)=u^k(x)+h\mathcal{P}\big(u^{k+1}(x),u^k(x)\big)\big(\psi_h(u^k(x))-u^k(x)\big), \tag{4.11}$$

where

$$\mathcal{P}\big(u^{k+1}(x),u^k(x)\big)=\mathcal{I}-\mathcal{P}_Y$$

with $\mathcal{P}_Y$ the orthogonal projection operator on the space

$$\begin{aligned}&Y\big(u^{k+1}(x),u^k(x)\big)\\ &=\operatorname{span}\Bigg\{1,\frac{u^{k+1}(x)+u^k(x)}{2},\\ &\qquad\frac{\alpha}{6}\big((u^{k+1}(x))^2+u^{k+1}(x)u^k(x)+(u^k(x))^2\big)+\frac{\nu}{2}\big(u_{xx}^{k+1}(x)+u_{xx}^k(x)\big)\Bigg\}.\end{aligned}$$

Remark 4.1. It is noted that the discrete variational derivative (2.6) may sometimes yield the same result as (2.7) for certain problems. We prefer the AVF-type discrete variational derivative (2.7) since the AVF-type integrator possesses several desirable properties, including linear covariance, automatic preservation of linear symmetries, and reversibility with respect to linear reversing symmetries [10]. Moreover, the expression (2.6) involves division by the difference $u^{k+1}(x)-u^k(x)$, which can lead to numerical instability when the solutions at consecutive time steps are close. In contrast, the AVF form (2.7) avoids this division and is numerically more robust and easier to handle in practical implementations.

4.2. Full discretization

To obtain fully discrete schemes for the KdV equation (4.1), finite-dimensional approximation in the spatial direction is required. In this section, we will demonstrate how the full-discretization scheme arises from the projection RK integrator (4.11). In what follows, we adopt the spectral framework from [2,4,5] to carry out the discretization in spatial direction.

First of all, we expand the solution $u(x,t)$ in space $L^2[-l,l]$ as

$$u(x,t)=\sum_{j\geq 0}u_j(t)\omega_j(x), \tag{4.12}$$

where

$$\omega_{2j}(x)=\sqrt{\frac{2-\delta_{j0}}{2l}}\cos\left(j\frac{x+l}{l}\pi\right),$$
$$\omega_{2j+1}(x)=\sqrt{\frac{1}{l}}\sin\left((j+1)\frac{x+l}{l}\pi\right),\quad j=0,1,2,\dots$$

is the orthonormal basis [2] satisfying

$$\int_{-l}^{l}\omega_i(x)\omega_j(x)\mathrm{d}x=\delta_{ij},\quad i,j=0,1,2,\dots$$

with δ_{ij} the Kronecker delta. Let

$$\boldsymbol{\omega}(x)=\begin{pmatrix}\omega_0(x)\\ \omega_1(x)\\ \omega_2(x)\\ \vdots\end{pmatrix},\quad \boldsymbol{u}(t)=\begin{pmatrix}u_0(t)\\ u_1(t)\\ u_2(t)\\ \vdots\end{pmatrix},$$

the expansion (4.12) can be written compactly as

$$u(x,t)=\boldsymbol{\omega}(x)^\top\boldsymbol{u}(t). \tag{4.13}$$

Correspondingly, let the expansions of $u^k(x)$ and $u^{k+1}(x)$ in (4.11) be

$$u^k(x)=\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k,\quad u^{k+1}(x)=\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1}. \tag{4.14}$$

It can be verified that

$$\boldsymbol{\omega}^{(k)}(x)=D^k\boldsymbol{\omega}(x),$$

where

$$D=\frac{\pi}{l}\begin{pmatrix}0 & & & \\ & 1\cdot J & & \\ & & 2\cdot J & \\ & & & \ddots\end{pmatrix}.$$

Here the skew-symmetric matrix J is defined as

$$J=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}=-J^\top.$$

Therefore, the projection RK integrator (4.11) now reads

$$\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1}=\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k+h\mathcal{P}\big(u^{k+1}(x),u^k(x)\big)\big(\psi_h(\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k)-\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k\big), \tag{4.15}$$

where

$$\mathcal{P}\big(u^{k+1}(x),u^k(x)\big)=\mathcal{I}-\mathcal{P}_Y$$

with $\mathcal{P}_Y$ the orthogonal projection operator on the space

$$\begin{aligned}
&Y\left(u^{k+1}(x),u^k(x)\right)\\
&=\text{span}\Big\{1,\boldsymbol{\omega}(x)^\top\frac{\boldsymbol{u}^{k+1}+\boldsymbol{u}^k}{2},\\
&\qquad\frac{\alpha}{6}\left((\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1})^2+\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1}\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k+(\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k)^2\right)\\
&\qquad+\frac{\nu}{2}\boldsymbol{\omega}(x)^\top(D^2)^\top(\boldsymbol{u}^{k+1}+\boldsymbol{u}^k)\Big\}\\
&=\boldsymbol{\omega}(x)^\top\text{span}\Big\{\boldsymbol{e},\frac{\boldsymbol{u}^{k+1}+\boldsymbol{u}^k}{2},\\
&\qquad\frac{\alpha}{6}\int_{-l}^{l}\boldsymbol{\omega}(x)((\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1})^2+\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1}\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k+(\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k)^2)dx\\
&\qquad+\frac{\nu}{2}(D^2)^\top(\boldsymbol{u}^{k+1}+\boldsymbol{u}^k)\Big\}
\end{aligned}$$

with $\boldsymbol{e}=(1,0,\dots,0,\dots)^\top$. Here, we have transferred the projection process in the space $L^2[-l,l]$ to the infinite dimensional vector space $\mathbb{R}^\infty$.

Bearing in mind the orthonormality of the basis functions $\omega_j(x)$, $j=0,1,\dots,$ it follows from (4.15) that the projection RK integrator can be expressed coordinate-wisely as

$$\boldsymbol{u}^{k+1}=\boldsymbol{u}^k+h(I-P)\left(\alpha\int_{-l}^{l}\boldsymbol{\omega}(x)\psi_h(\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k)dx-\boldsymbol{u}^k\right),\tag{4.16}$$

where I is the infinite dimensional identity matrix and P is the projection matrix on the subspace

$$\begin{aligned}
&\text{span}\Big\{\boldsymbol{e}_1,\frac{\boldsymbol{u}^{k+1}+\boldsymbol{u}^k}{2},\\
&\qquad\frac{\alpha}{6}\int_{-l}^{l}\boldsymbol{\omega}(x)((\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1})^2+\boldsymbol{\omega}(x)^\top\boldsymbol{u}^{k+1}\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k+(\boldsymbol{\omega}(x)^\top\boldsymbol{u}^k)^2)dx\\
&\qquad+\frac{\nu}{2}(D^2)^\top(\boldsymbol{u}^{k+1}+\boldsymbol{u}^k)\Big\},
\end{aligned}\tag{4.17}$$

which can be calculated as

$$P=G(G^\top G)^{-1}G^T,\tag{4.18}$$

where G be a $\infty\times 3$ matrix whose columns consist of the bases of the subspace (4.17).

Then, suitable truncation leads to the concrete practical full-discretization projection RK schemes. To be more precisely, we restrict ourselves to the $(2N+1)$-dimension subspace $\mathcal{V}_N=\text{span}\{\omega_j(x),j=0,1,\dots,2N\}$ and look for the approximation

$$u(x,t)\approx u_{2N+1}(x,t)=\boldsymbol{\omega}_{2N+1}^\top(x)\boldsymbol{u}_{2N+1}(t)\tag{4.19}$$

with

$$\boldsymbol{\omega}_{2N+1}(x) = \begin{pmatrix} \omega_0(x) \\ \omega_1(x) \\ \vdots \\ \omega_{2N}(x) \end{pmatrix} \in \mathbb{R}^{2N+1}, \quad \boldsymbol{u}_{2N+1}(t) = \begin{pmatrix} u_0(t) \\ u_1(t) \\ \vdots \\ u_{2N}(t) \end{pmatrix} \in \mathbb{R}^{2N+1}.$$

The truncated projection RK integrator in space $\mathcal{V}_N$ can be expressed coordinate-wisely as

$$\begin{aligned} \boldsymbol{u}_{2N+1}^{k+1} = \boldsymbol{u}_{2N+1}^{k} &+ \Delta t (I_{2N+1} - P_{2N+1}) \\ &\times \left(\alpha \int_{-l}^{l} \boldsymbol{\omega}_{2N+1}(x) \psi_h(\boldsymbol{\omega}_{2N+1}(x)^\top \boldsymbol{u}_{2N+1}^k) dx - \boldsymbol{u}_{2N+1}^k \right), \end{aligned} \tag{4.20}$$

where I_{2N+1} is the $(2N+1)$-dimensional identity matrix,

$$D_{2N+1} = \frac{\pi}{l} \begin{pmatrix} 0 & & & \\ & 1 \cdot J & & \\ & & \ddots & \\ & & & N \cdot J \end{pmatrix} \in \mathbb{R}^{(2N+1)\times(2N+1)}$$

and

$$P_{2N+1} = G_{2N+1}(G_{2N+1}^\top G_{2N+1})^{-1} G_{2N+1}^T \tag{4.21}$$

with G_{2N+1} be a $(2N+1) \times 3$ matrix whose columns consist of the bases of the $2N+1$ dimensional truncation of the subspace (4.17).

Similar to the projection RK integrator in the space $L^2[-l, l]$, we have the following result for the truncated projection RK integrator (4.20) concerning about the preservation of the invariants.

Theorem 4.1. *The truncated projection RK integrator* (4.20) *preserves exactly the truncated mass*

$$M_{2N+1} = \int_{-l}^{l} \boldsymbol{\omega}_{2N+1}^\top(x) \boldsymbol{u}_{2N+1} \, \mathrm{d}x, \tag{4.22}$$

the truncated momentum

$$K_{2N+1} = \int_{-l}^{l} \left(\boldsymbol{\omega}_{2N+1}^\top(x) \boldsymbol{u}_{2N+1} \right)^2 \mathrm{d}x. \tag{4.23}$$

and the truncated energy

$$H_{2N+1} = \int_{-l}^{l} \frac{1}{6} \alpha \big(\boldsymbol{\omega}_{2N+1}^\top(x) \boldsymbol{u}_{2N+1} \big)^3 - \frac{1}{2} \nu \big(\boldsymbol{\omega}_{2N+1}^\top(x) D_{2N+1}^\top \boldsymbol{u}_{2N+1} \big)^2 \mathrm{d}x. \tag{4.24}$$

In the following, we numerically solve a KdV equation using the truncated projection RK integrator (4.20) with different stepsizes to confirm the theoretical results.

Problem 4.1. Consider the interaction of two solitary waves which are modeled by the KdV equation (4.1) with the initial condition

$$u_0(x) = \frac{12}{(1+e^{\theta_1}+e^{\theta_2}+a^2e^{\theta_1+\theta_2})^2} \times \Big[k_1^2e^{\theta_1}+k_2^2e^{\theta_2}+2(k_2-k_1)^2e^{\theta_1+\theta_2}+a^2\big(k_2^2e^{\theta_1}+k_1^2e^{\theta_2}\big)e^{\theta_1+\theta_2}\Big],$$

where

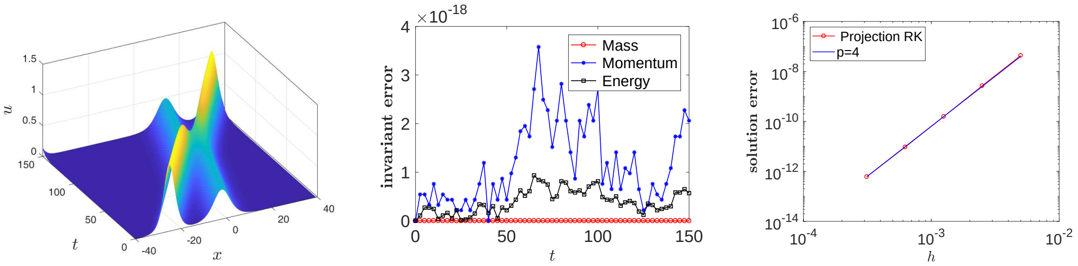
$$a^2 = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \frac{1}{25}, \qquad \theta_1 = k_1x+x_1, \qquad \theta_2 = k_2x+x_2.$$

In this problem, we set $k_1 = 0.4, k_2 = 0.6, x_1 = 4, x_2 = 15$. This problem is derived from [42]. The parameters in the KdV equation are chosen as $\alpha = -1, \nu = -1$ and the solution region as $x \in [-40, 40]$.

We integrate the KdV equation in the interval $t \in [0, 150]$ with $N = 2^6$ and $h = 0.005$. The fourth-order RK integrator with Butcher tableau

0				
1/2	1/2			
1/2	0	1/2		
1	0	0	1	
	1/6	2/6	2/6	1/6

is chosen as the underlying integrator. The numerical solution obtained by the truncated projection RK integrator and the preservation of three invariants are shown in Figs. 1(a)-1(b). It is observed that the three truncated invariants are preserved by the numerical integrator and the numerical solution is well performed. The two solitary waves move at a constant speed. The velocity of the taller solitary wave is greater than that of the shorter one. At $t = 80$, the two solitons overlap, and they are completely apart at $t = 120$, having swapped their positions.



(a) Numerical solution (b) Invariants preservation (c) Algebraic order

Figure 1: Numerical results for Problem 4.1 with $N = 2^6$. (a) the numerical solution obtained by truncated projection RK integrator; (b) preservation of the three truncated invariants (4.22), (4.23) and (4.24); (c) order of convergence.

Moreover, we integrate the KdV equation in the interval $t \in [0,1]$ using the truncated projection RK integrator with different stepsizes. The solution errors versus the stepsizes are displayed in Fig. 1(c). It is noted here that since the exact solution for the KdV equation (4.1) cannot be obtained, the reference solution is computed by using the underlying fourth-order RK integrator with a very small time stepsize $h_{\text{ref}} = h/10$, where h is the smallest time stepsize used in our test. This ensures that the error in the reference solution is negligible compared to the errors of the method being tested. It can be seen from the numerical result that the projection RK integrator maintains the algebraic order of the underlying RK integrator.

5. Conclusions and remarks

In the present paper, by introducing the concept of discrete variational derivative, we obtain a semi-analytical energy-preserving discrete variational derivative integrator for Hamiltonian PDEs, which can be viewed as a generalization of the discrete gradient for Hamiltonian ODEs. Furthermore, semi-analytical multiple invariants-preserving integrators for conservative PDEs are constructed by projection. In this paper, we focus ourselves on the temporal direction, the obtained integrators are time-stepping. One more step of a finite-dimension discretization in spatial direction (including suitable approximation to the partial derivatives ∂_x, ∂_{xx} etc.) will lead to a full-discretization schemes for the conservative PDEs (2.1). All the analysis in the paper makes perfect sense after replacing $u^k(x)$ by the finite-dimension vector $\mathbf{u}^k$ and the continuous L^2 inner product by the discrete l^2 inner product. This paper offers a new framework for the constructing multiple invariants-preserving integrators for conservative PDEs. The novel approach is conceptually simple, versatile, and helpful for the theoretical analysis of full-discretization energy-preserving schemes.

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