A novel discrete variational derivative method using “average-difference methods”

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Abstract

We consider conservative numerical methods for a certain class of PDEs, for which standard conservative methods are not effective. There, the standard skew-symmetric difference operators indispensable for the discrete conservation law cause undesirable spatial oscillations. In this letter, to circumvent this difficulty, we propose a novel “average-difference method,” which is tougher against such oscillations. However, due to the lack of the apparent skew-symmetry, the proof of the discrete conservation law becomes nontrivial. In order to illustrate partially the superiority, we compare the standard and proposed methods for the linear Klein–Gordon equation.

Keywords geometric integration, conservative systems, Klein–Gordon equation

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1. Introduction

This letter is a prompt report on the numerical integration of the partial differential equation (PDE) in the form

$$u_{tx} = \frac{\delta G}{\delta u}, \quad \mathcal{H}(u) := \int_0^L G(u, u_x, \dots) dx, \quad (1)$$

where subscripts t or x denote the partial differentiation with respect to t or x , and $\delta G/\delta u$ is the variational derivative of G . We assume the periodic boundary condition $u(t, x+L) = u(t, x)$ ($\forall t \in \mathbb{R}_+ := [0, +\infty)$, $\forall x \in \mathbb{R}$), where $L \in \mathbb{R}_+$ is a constant. When the derivatives of u do not appear in $\mathcal{H}$, the equation (1) is called the (nonlinear) Klein–Gordon (KG) equation in light-cone coordinates. In particular, if $G(u) = -\cos u$ (i.e., $\delta G/\delta u = \sin u$), it is called the sine-Gordon equation. Moreover, the class of PDEs in the form (1) is closely related to the Ostrovsky equation [1], the short pulse equation [2], etc. For their numerical treatments, due to the possible indefiniteness caused by the spatial derivative in the left-hand side, it seems a systematic numerical framework for (1) is yet to be investigated, though a few exceptions for specific cases can be found (e.g., [3, 4]).

In this letter, we focus on conservative methods. Under the periodic boundary condition, the target equation (1) has the conserved quantity $\mathcal{H}$:

$$\begin{aligned} \frac{d\mathcal{H}}{dt} &= \int_0^L \frac{\delta G}{\delta u} u_t dx = \int_0^L u_{tx} u_t dx \\ &= [u_t^2]_0^L - \int_0^L u_t u_{tx} dx = - \int_0^L u_t u_{tx} dx = 0. \end{aligned} \quad (2)$$

Note that the skew-symmetry of the differential operator $\partial_x := \partial/\partial x$ is crucial here. A numerical scheme is called

conservative when it replicates such a conservation property (see, e.g., [5, 6]). The numerical solutions obtained by such schemes are often more stable than those of general-purpose methods. There, the crucial point for the discrete conservation law is the skew-symmetry of the difference operator, which corresponds to that of the differential operator; when one tries to construct a conservative finite-difference scheme for the equation (1), the differential operator ∂_x in left-hand side must be replaced by one of the skew-symmetric difference operators, for example, the central difference operators, the compact finite difference operators (see, e.g., Kanazawa–Matsuo–Yaghchi [7]), and the Fourier-spectral difference operator (see, e.g., Fornberg [8]). This is intrinsically indispensable, at least to the best of the present authors’ knowledge. This, however, at the same time, leads to an undesirable side effect that the numerical solutions tend to suffer from spatial oscillations. Although this tendency has been observed in various PDEs in the literature, the situation becomes far serious in the nonlinear PDEs of the form (1). For example, one observes dreadful spatial oscillations in the sine-Gordon equation (see, [9, Fig. 14]).

In this letter, to work around this difficulty, we propose a novel “average-difference method,” which is tough against such undesirable spatial oscillations for the PDEs in the form (1) (see, [9, Fig. 16]). A similar method has been, in fact, already investigated by Nagisa [10]. However, he used this method for advection-type equations, and concluded the method was unfortunately not more advantageous than existing methods. In this letter, we instead construct an average-difference method for the PDE (1), and combine it with the idea of conservation mentioned above. The discrete conserva-

tion law (Theorem 2) of the average-difference method is the main result of this letter; note that since the proposed method loses the apparent skew-symmetry, its proof becomes rather nontrivial than that of the standard conservative method (Proposition 1).

Then, as a first step of understanding the good behavior of the proposed method (observed in the sine-Gordon case [9], for example), we consider the linear Klein–Gordon (KG) equation, which is the simplest case with $G(u) = u^2/2$. There, we theoretically observe the discrepancy in the phase speeds of high frequency components, which well describes the actual numerical behaviors.

2. The standard conservative method

The conservative scheme for the PDE (1) can be constructed in the spirit of the discrete variational derivative method (DVDM) (see, the monograph [5] for details). There, one utilizes the concept of the “discrete variational derivative” and skew-symmetric difference operators. The symbol $u_k^{(m)}$ denotes the approximation $u_k^{(m)} \approx u(m\Delta t, k\Delta x)$ ($m = 0, \dots, M; k \in \mathbb{Z}$), where Δt and Δx ($:= L/K$) are the temporal and spatial mesh sizes, respectively. Here, we assume the discrete periodic boundary condition $u_{k+K}^{(m)} = u_k^{(m)}$ ($k \in \mathbb{Z}$), and thus, we use the notation $u^{(m)} := (u_1^{(m)}, \dots, u_K^{(m)})^\top$. Let us introduce the spatial central difference operator $\delta_x^{(1)}$ and the temporal forward difference operator δ_t^+ :

$$\delta_x^{(1)} u_k^{(m)} = \frac{u_{k+1}^{(m)} - u_{k-1}^{(m)}}{2\Delta x}, \quad \delta_t^+ u_k^{(m)} = \frac{u_k^{(m+1)} - u_k^{(m)}}{\Delta t}.$$

The discrete counterpart $\mathcal{H}_d$ of the functional $\mathcal{H}$ can be defined as

$$\mathcal{H}_d(u^{(m)}) := \sum_{k=1}^K G_d(u_k^{(m)}) \Delta x,$$

where $G_d(u_k^{(m)})$ is an appropriate approximation of $G(u, u_x, \dots)$. Then, the discrete variational derivative $\delta G_d / \delta(u^{(m+1)}, u^{(m)})_k$ is defined as a function satisfying

$$\delta_t^+ \mathcal{H}_d(u_k^{(m)}) = \sum_{k=1}^K \frac{\delta G_d}{\delta(u^{(m+1)}, u^{(m)})_k} \delta_t^+ u_k^{(m)} \Delta x. \quad (3)$$

For the construction of such one, see [5]. By using the discrete variational derivative, we can construct a conservative scheme

$$\delta_x^{(1)} \delta_t^+ u_k^{(m)} = \frac{\delta G_d}{\delta(u^{(m+1)}, u^{(m)})_k}. \quad (4)$$

As stated in the introduction, the key ingredient here is the skew-symmetry of the central difference operator.

Note that whether the scheme (4) (and (5) in the next section) is (uniquely) solvable or not depends on the concrete form of G (see, e.g., [5] for mathematical analysis of other type of PDEs). Another note should go to the fact that the mathematical analysis of the finite difference methods for the PDEs in the form (1) on the periodic domain seems to be nontrivial due to the singularity of the difference operator in the left-hand side. Below we

show the conservation property assuming the solvability. This note also applies to the next section.

Proposition 1 *Suppose the numerical scheme (4) has a solution $u_k^{(m)}$ under the periodic boundary condition. Then, it satisfies $\mathcal{H}_d(u^{(m+1)}) = \mathcal{H}_d(u^{(m)})$.*

Proof Thanks to the definition (3) of the discrete variational derivative, we can follow the line of the discussion (2) as follows:

$$\begin{aligned} \delta_t^+ \mathcal{H}_d(u^{(m)}) &= \sum_{k=1}^K \frac{\delta G_d}{\delta(u^{(m+1)}, u^{(m)})_k} \delta_t^+ u_k^{(m)} \Delta x \\ &= \sum_{k=1}^K \left(\delta_x^{(1)} \delta_t^+ u_k^{(m)} \right) \delta_t^+ u_k^{(m)} \Delta x, \end{aligned}$$

whose right-hand side vanishes due to the skew-symmetry of the central difference operator $\delta_x^{(1)}$:

$$\sum_{k=1}^K u_k \delta_x^{(1)} v_k \Delta x = - \sum_{k=1}^K \left(\delta_x^{(1)} u_k \right) v_k \Delta x$$

holds for any $u, v \in \mathbb{R}^K$.

(QED)

The discrete conservation law can also be proved similarly for the other skew-symmetric difference operators including Fourier-spectral difference operator.

3. “Average-difference method”

In this section, we propose the novel method. There, instead of the single skew-symmetric difference operator, we employ the pair of the forward difference and average operators:

$$\delta_x^+ u_k^{(m)} = \frac{u_{k+1}^{(m)} - u_k^{(m)}}{\Delta x}, \quad \mu_x^+ u_k^{(m)} = \frac{u_{k+1}^{(m)} + u_k^{(m)}}{2}.$$

The average-difference method for the equation (1) can be written in the form

$$\delta_x^+ \delta_t^+ u_k^{(m)} = \mu_x^+ \frac{\delta G_d}{\delta(u^{(m+1)}, u^{(m)})_k}. \quad (5)$$

The name “average-difference” comes from the idea of approximating ∂_x with the pair of (δ_x^+, μ_x^+) ; this makes sense for more general PDEs, and thus is independent of any conservation properties. Still, in this letter we focus on (1) and (5).

Although it is constructed in the spirit of DVDM, now the forward difference operator δ_x^+ loses the apparent skew-symmetry, and accordingly, the proof of the discrete conservation law becomes unobvious. A similar proof can be found in Nagisa [10]. Note that the numerical scheme (5) and its discrete conservation law below are valid for general nonlinear PDE (1).

Theorem 2 *Suppose the average-difference method (5) has a solution $u_k^{(m)}$ under the periodic boundary condition. Then, it satisfies $\mathcal{H}_d(u^{(m+1)}) = \mathcal{H}_d(u^{(m)})$.*

Proof By using the definition (3) of the discrete variational derivative, we see that

$$\delta_t^+ \mathcal{H}_d(u^{(m)}) = \sum_{k=1}^K \frac{\delta G_d}{\delta(u^{(m+1)}, u^{(m)})_k} \delta_t^+ u_k^{(m)} \Delta x.$$

Here, for brevity, we introduce the notation

$$a_k = \frac{\delta G_d}{\delta(u^{(m+1)}, u^{(m)})_k}, \quad b_k = \delta_t^+ u_k^{(m)}.$$

Note that the equation (5) implies the relation $\delta_x^+ b_k = \mu_x^+ a_k$. By using the identity

$$\begin{aligned} & \frac{\alpha^+ \beta^+ + \alpha \beta}{2} \\ &= \left(\frac{\alpha^+ + \alpha}{2} \right) \left(\frac{\beta^+ + \beta}{2} \right) + \frac{1}{4} (\alpha^+ - \alpha) (\beta^+ - \beta), \end{aligned}$$

which holds for any $\alpha, \alpha^+, \beta, \beta^+ \in \mathbb{R}$, we see

$$\begin{aligned} \sum_{k=1}^K a_k b_k &= \sum_{k=1}^K \frac{a_{k+1} b_{k+1} + a_k b_k}{2} \\ &= \sum_{k=1}^K \left[(\mu_x^+ a_k) (\mu_x^+ b_k) + \frac{\Delta x^2}{4} (\delta_x^+ a_k) (\delta_x^+ b_k) \right] \\ &= \sum_{k=1}^K \left[(\delta_x^+ b_k) (\mu_x^+ b_k) + \frac{\Delta x^2}{4} (\delta_x^+ a_k) (\mu_x^+ a_k) \right] \\ &= \sum_{k=1}^K \left[\frac{1}{2} \left(\delta_x^+ b_k^2 + \frac{\Delta x^2}{4} \delta_x^+ a_k^2 \right) \right] = 0, \end{aligned}$$

which proves the theorem.

(QED)

4. Example: linear KG equation

In this section, in order to illustrate partially the cause of the superiority of the proposed method, we focus on the simplest case, the linear Klein–Gordon equation

$$u_{tx} = \frac{\delta G}{\delta u} = u, \quad \mathcal{H}(u) := \frac{1}{2} \int_0^{2\pi} u^2 dx \quad (6)$$

under the periodic domain with the period $L = 2\pi$. The exact solution of the linear Klein–Gordon equation (6) can be formally written in the form

$$u(t, x) = \sum_{n \in \mathbb{Z} \setminus \{0\}} a_n \exp\left(-i \frac{t}{n}\right) \exp(inx), \quad (7)$$

where i is the imaginary unit, and $a_n \in \mathbb{C}$ is determined by the initial condition $u(0, x) = u_0(x)$:

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} u_0(x) \exp(-inx) dx.$$

4.1 Numerical experiment

In this section, we conduct a numerical experiment under the initial condition

$$u_0(x) = \begin{cases} 1 & (\pi/2 < x < 3\pi/2), \\ -1 & (0 \leq x \leq \pi/2 \text{ or } 3\pi/2 \leq x < 2\pi). \end{cases}$$

The corresponding solution can be formally written as

$$u(t, x) = \sum_{n=1}^{\infty} \left(-\frac{4}{n\pi} \sin \frac{n\pi}{2} \right) \cos \left(nx - \frac{t}{n} \right).$$

Figs. 1 and 2 show the numerical solutions of the central difference scheme $\delta_x^{(1)} \delta_t^+ u_k^{(m)} = \mu_t^+ u_k^{(m)}$ and the

Fig. 1. The numerical solution of the central difference scheme ($K = 129, \Delta t = 0.01$).

Fig. 2. The numerical solution of the average-difference scheme ($K = 129, \Delta t = 0.01$).

Fig. 3. The comparison of the numerical solutions at $t = 50$ ($K = 129, \Delta t = 0.01$). The black dotted line represents the exact solution. The green, blue, and red solid lines denote the numerical solution of the central difference, the Fourier-spectral difference, and the average-difference method, respectively.

average-difference method $\delta_x^+ \delta_t^+ u_k^{(m)} = \mu_x^+ \mu_t^+ u_k^{(m)}$ under the discrete periodic BC $u_{k+K}^{(m)} = u_k^{(m)}$ ($L = K\Delta x$) and the initial condition $u_k^{(0)} = u_0(k\Delta x)$. Each numerical scheme is a special case of the conservative method described in the previous sections; when one define $G_d(u_k^{(m)}) := (u_k^{(m)})^2/2$, $\mu_t^+ u_k^{(m)}$ is the discrete variational derivative. It is easy to verify that these schemes are uniquely solvable for any Δt and Δx .

As shown in Fig. 1, the central difference scheme suffers from the spatial oscillation, whereas the proposed method reproduces the smooth profiles until $t = 1$ (Fig. 2). When we employ the Fourier-spectral difference δ_{PS} (see, e.g., [8] for the definition) instead of the central difference, i.e., $\delta_{PS} \delta_t^+ u_k^{(m)} = \mu_t^+ u_k^{(m)}$, the numerical

solution does not suffer from visible spatial oscillation until $t = 1$ (the profile is omitted since it is quite similar to Fig. 2).

However, as shown in Fig. 3, which shows the numerical solutions of each scheme at $t = 50$, the Fourier-spectral scheme also suffers from the undesirable spatial oscillation, whereas the proposed average-difference method reproduces a better profile. This could be attributed to the fact that the Fourier-spectral difference can be regarded as a higher-order central difference, and thus should share the same property to a certain extent.

These observations are consistent with the instability in the nonlinear (sine-Gordon) case [9].

4.2 Comparison of phase speeds

In order to clarify the difference between the standard conservative method and proposed method, we consider the following three semi-discretizations

$$\delta_x^{(1)} \dot{u}_k = u_k, \quad (8)$$

$$\delta_{\text{PS}} \dot{u}_k = u_k, \quad (9)$$

$$\delta_x^+ \dot{u}_k = \mu_x^+ u_k, \quad (10)$$

where $u_k(t) \approx u(t, k\Delta x)$ for $k \in \mathbb{Z}$ ($u_{k+K} = u_k$). Note that, the implicit midpoint method for the semi-discretizations above coincide with the numerical schemes used in the previous section.

In view of the superposition principle, we deal with the single component $\exp(-it/n) \exp(inx)$ ($n \in \mathbb{Z} \setminus \{0\}$) of the solution (7). Thus, we consider the solution of the semi-discretizations above in the form $u_k = \exp(ic_n t) \exp(ink\Delta x)$ ($c_n \in \mathbb{R}$) for each $n \in \{m \in \mathbb{Z} \mid 2m/K \notin \mathbb{Z}\}$, which gives an exact solutions of (8), (9), and (10) with appropriate choices of c_n . For the central difference scheme (8), we see

$$c_n^{\text{CD}} = -\frac{\Delta x}{\sin n\Delta x}.$$

If we employ the Fourier-spectral difference operator instead of the central difference, we see

$$c_n^{\text{PS}} = -\frac{1}{n} \quad (|n| < K/2),$$

and $c_{n+K} = c_n$ holds for any $n \in \{m \in \mathbb{Z} \mid 2m/K \notin \mathbb{Z}\}$. For the average-difference scheme (10), we obtain

$$c_n^{\text{AD}} = -\frac{\Delta x}{2 \tan(n\Delta x/2)}.$$

The phase speeds c_n corresponding to each numerical scheme are summarized in Fig. 4 ($K = 65$). As shown in Fig. 4, the phase speed of the central difference scheme (8) are falsely too fast for high frequency components ($n \approx K/2$). On the other hand, the errors of the phase speeds of the average-difference method are much smaller. This discrepancy in phase speeds of high frequency component is the cause of the superiority of the proposed method in comparison with the central difference method (Fig. 3).

5. Concluding remarks

The results above can be extended in several ways. First, instead of the cumbersome proof in Theorem 2, we

Fig. 4. The phase speeds for each $n = 1, 2, \dots, 32$ ($K := 65$). The red circles, blue crosses, and green triangles correspond to the average-difference, Fourier-spectral difference, and central difference schemes, respectively.

can introduce the concept of generalized skew-symmetry, by which a more sophisticated “average-difference” version of the DVDM could be given. Second, we should try more general PDEs to see to which extent the new DVDM is advantageous. Third, as noted before the Proposition 1, the mathematical analysis of the numerical methods for the PDEs in the form (1) should be done. Finally and ultimately, we hope to construct a systematic numerical framework for (1), based on the above observations. The authors have already got some results on these issues, which will be reported somewhere soon.

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