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with a Mixed Derivative

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ABSTRACT. Recently, various evolutionary partial differential equations (PDEs) with a mixed derivative have been emerged and drawn much attention. However, their theoretical and numerical studies are still in their early stage. In this paper, we mainly focus on numerical treatment, and as a first step to construct a unified framework for such PDEs, we propose a procedure that transform the PDEs with a mixed derivative into a standard form that suits some analysis. Then, based on the procedure, we classify and discuss the spatial discretizations. As a result, we show the average-difference method is suitable for the discretization of the mixed derivative, and furthermore newly introduce its higher order extensions that opens a new door for accurate computations of such PDEs.

1. INTRODUCTION

In this paper, we consider numerical methods for the initial value problem for the evolutionary partial differential equations (PDEs) in the form

$$
(1.1) \qquad \begin{cases} (u_t + g(u, u_x, u_{xx}, \dots))_x = f(u, u_x, u_{xx}, \dots) & (t \in [0, T], x \in \mathbb{S}), \\ u(0, x) = u_0(x) & (x \in \mathbb{S}), \end{cases}
$$

on the periodic domain $\mathbb{S} = \mathbb{R}/2\pi\mathbb{Z}$. Here, $u : [0, T] \times \mathbb{S} \to \mathbb{R}$ is a dependent variable, t and x are temporal and spatial independent variables, subscripts t and x denote the partial derivative with respect to t and x, and u_0 is an initial condition. Various equations in the form (1.1) have been recently emerged and lively studied (see, Section 3 for examples and related results on them). However, theoretical and numerical treatments of them are more difficult than usual evolutionary equations due to the presence of the spatial differential operator $\partial_x := \partial/\partial x$ operating on u_t. We call the resulting term u_{tx} *mixed derivative* hereafter.

The spatial differential operator ∂_x in the mixed derivative is not invertible under the standard setting of the space of periodic functions such as the Sobolev spaces (the precise meaning will be explained in Section 2). Therefore, some problems in the form (1.1) are underdetermined while the others are well-posed. In this paper, we focus on the latter case. Moreover, we restrict ourselves to the spatial discretization (see, Remark 1.3), because the biggest issue is how to treat the spatial differential operator operating on u_t. In view of this, we mean the operator on u_t when we merely say "the spatial differential operator," although other spatial differential operators can appear in the problem (1.1) in the functions g and f.

Before stating our challenge in this paper, we first note that there are existing works for similar initial value problems on the whole real line with the vanishing boundary conditions. Since the spatial differential operator ∂_x is invertible when regarded as a linear operator between some appropriate function spaces (see, e.g., Iório–Nunes [23] and references therein), the initial value problem can be equivalently transformed into that for the integro-differential equation in the form

$$u_t + g(u, u_x, u_{xx}, \dots) = \partial_x^{-1} f(u, u_x, u_{xx}, \dots)$$

(see, e.g., [29, 30, 7] for examples). Here, the operator

$$\partial_x^{-1} v(x) = \frac{1}{2} \left(\int_{-\infty}^x v(y) \mathrm{d}y - \int_x^\infty v(y) \mathrm{d}y \right)$$

is the inverse of the spatial differential operator (the inverse operator ∂_x^{-1} is sometimes called as the antiderivative). We call the original differential equation *differential form*, and the induced integro-differential equation *integral form*. Their integral forms have often been utilized rather than differential forms (see, e.g., [28, 7]) in order to prove the well-posedness of the equations with a mixed derivative on the whole real line. It should be noted that the situation is similar if one deal with a finite interval with the Dirichlet boundary condition, where again ∂_x is (in some sense) invertible.

However, due to the lack of the invertibility of ∂_x, the derivation of the integral form is challenging when we deal with the periodic domain. One usually hope to impose the periodic boundary conditions on a finite interval in order to conduct some numerical experiments, because the class of PDEs with a mixed derivative involves a lot of equations modeling the propagation of various waves.

Though there is certainly no unified approach so far to derive the integral form on the periodic domain, there are some simple exceptions. For example, the reduced Ostrovsky equation

$$(1.2) \qquad \left(u_t - \left(\frac{1}{2} u^2 \right)_x \right)_x = \gamma u.$$

It models water waves on a very shallow rotating fluid, and is also referred as the short wave equation [22], Ostrovsky–Hunter equation [4], Vakhnenko equation [45], and Ostrovsky–Vakhnenko equation [5].

For this equation, Hunter [22] derived the integral form

$$(1.3) \qquad u_t - \left(\frac{1}{2} u^2 \right)_x = \gamma \left(\int_0^x u(t, y) \mathrm{d}y - \frac{1}{2\pi} \int_{\mathbb{S}} \int_0^z u(t, y) \mathrm{d}y \mathrm{d}z \right).$$

As the present authors understand, the transformation above can be described as follows (there is no explicit explanation on it in Hunter [22]). Let $u \in C([0, T]; H^2(\mathbb{S})) \cap C^1([0, T]; H^1(\mathbb{S}))$ be a solution of the differential form (1.2) (see, [30, Lemma 1]), where $H^s(\mathbb{S})$ denotes the sth Sobolev space with the standard inner product ($u(t)$ denotes a function satisfying $(u(t))(x) = u(t, x)$ for any $x \in \mathbb{S}$, and we use similar notation hereafter). Here, the spatial differential operator operating on $u_t - (u^2/2)_x$ can be regarded as a linear operator whose domain is $H^1(\mathbb{S})$, and is not invertible as is. Therefore, we consider a restriction of its domain into an appropriate linear subspace $A \subseteq H^1(\mathbb{S})$ such that (a) $u_t - (u^2/2)_x \in A$ holds and (b) the restricted operator $\partial_x|A$ is invertible. Fortunately, for the reduced Ostrovsky equation, the set $\check{H}^1(\mathbb{S})$ of zero-mean functions, i.e., $\check{H}^1(\mathbb{S}) = \{ v \in H^1(\mathbb{S}) \mid \int_{\mathbb{S}} v(x) \mathrm{d}x = 0 \}$, satisfies these two conditions. The latter condition (b) can be easily verified. For (a), we first note that the integral of the both sides of (1.2) over x yields $\int_{\mathbb{S}} u(t, x) \mathrm{d}x = 0$, which implies $\int_{\mathbb{S}} u_t(t, x) \mathrm{d}x = 0$. In other words, $u_t(t) \in \check{H}^1(\mathbb{S})$ holds for any $t \in [0, T]$ (this can also be regarded as the consequence of the solution $u(t)$ being an orbit on the linear subspace $\check{H}^1(\mathbb{S})$). Since $(u^2/2)_x \in \check{H}^1(\mathbb{S})$ also holds due to the periodicity, the former condition (a) is also satisfied. From the observation above, ∂_x operating on $u_t - (u^2/2)_x$ can be regarded as the restricted operator $\check{\partial}_x := \partial_x|\check{H}^1(\mathbb{S})$, and the differential form (1.2)

can be rewritten as

$$\check{\partial}_x \left(u_t - \left(\frac{1}{2} u^2 \right)_x \right) = \gamma u.$$

Since $\check{\partial}_x$ is invertible, by operating with $\check{\partial}_x^{-1}$ concretely defined as

$$(1.4) \qquad \check{\partial}_x^{-1} v(x) = \int_0^x v(y) \mathrm{d}y - \frac{1}{2\pi} \int_{\mathbb{S}} \int_0^z v(y) \mathrm{d}y \mathrm{d}z,$$

we obtain

$$u_t - \left(\frac{1}{2} u^2 \right)_x = \gamma \check{\partial}_x^{-1} u,$$

which coincides with the integral form (1.3).

It should be noted that though the operator $\check{\partial}_x^{-1}$ (more precisely its concrete form (1.4)) had been employed in the literature for deriving the integral forms of various equations in addition to the reduced Ostrovsky equation above, no one has clarified the class of equations to which this strategy can be applicable (this issue will be discussed later). Another note should go to the fact that this operator is often denoted by ∂_x^{-1} (see, e.g., [46, 31, 30]). However, we prefer to employ the somewhat unusual notation $\check{\partial}_x^{-1}$ in order to clarify in which sense this operator is the inverse of the spatial differential operator. Related to this, though $\check{\partial}_x^{-1}$ is sometimes called as an "antiderivative," we do not use this terminology that allows the ambiguity.

Based on the integral form derived by Hunter [22], various studies on the reduced Ostrovsky equation have been conducted. Hunter [22] himself conducted numerical experiments based on the integral form (however, the discrete counterpart of the operator $\check{\partial}_x^{-1}$ is not written). Liu–Pelinovsky–Sakovich [30] conducted numerical experiments by the pseudospectral method. Coclite–Ridder–Risebro [8] devised a numerical scheme based on the integral form (1.3) by using the trapezoidal rule for the discretization of the operator $\check{\partial}_x^{-1}$. Liu–Pelinovsky–Sakovich [30] showed the local well-posedness and the condition of the finite-time wave breaking. Coclite–Ridder–Risebro [8] showed the unique existence of the entropy solution. Moreover, they also proved that the numerical solution obtained by their method converges to the unique entropy solution.

Let us turn our attention to existing works on other equations with a mixed derivative (note that, we focus on the results on the periodic domain unless otherwise stated). Although there are sporadic studies for some specific cases of (1.1), including (1.2) we have already seen, the discussion on this class of PDEs from a unified viewpoint is still missing. First of all, note that, in view of the history of the studies on the reduced Ostrovsky equation, we think that studies on each specific case of (1.1) should be done in the following order: (i) find a transformation into a integral form, (ii) construct numerical schemes based on the integral form, (iii) prove the well-posedness of the initial value problem, and (iv) conduct some mathematical analyses on the numerical schemes. In this sense, PDEs in (1.1) can be classified into the following four classes, based on to which extent they are investigated (see, Table 1):

(I): The case with $g = h_x(u)$ and $f(u) = u$, i.e.,

$$(1.5) \qquad (u_t + h_x(u))_x = u.$$

(II): The case with $g = h_x(u, u_x, \dots)$ and $f(u) = u$, i.e.,

$$(1.6) \qquad (u_t + h_x(u, u_x, \dots))_x = u.$$

(III): The case with g: general, $f(u) = u$, i.e.,

$$(1.7) \qquad (u_t + g(u, u_x, \dots))_x = u.$$

(IV): The general case, i.e.,

$$(1.8) \qquad (u_t + g(u, u_x, \dots))_x = f(u, u_x, \dots).$$

TABLE 1. Existing results on the initial value problem (1.1). (A) and (B) indicate results newly obtained in this paper. The blank cell implies that there are no results even for a specific case.

	Class	(I)	(II)	(III)	(IV)
	Implicit constraint	Linear			Nonlinear
(i)	Integral form	[22]	[46],[32],...	[31]	(A)
(ii)	Discretization	[29, 30],[8],...	[46],[32],...	(B)	(B)
(iii)	Well-posedness	[29, 30],[8]			
(iv)	Mathematical analysis of discretization	[8]			

Section 3 is devoted to list the examples of each class and existing works on them.

It should be noted that, equations in the class (IV) have the implicit constraint $\mathcal{F}(u(t)) = 0$, where

$$(1.9) \qquad \mathcal{F}(v) = \int_{\mathbb{S}} f(v, v_x, \dots) \mathrm{d}x.$$

Recall that, the linear implicit constraint $\int_{\mathbb{S}} u(t, x) \mathrm{d}x = 0$ is satisfied for any solutions of the reduced Ostrovsky equation (1.2), included in the class (I). Actually, equations in the class (I), (II), and (III) have the same linear implicit constraint, and thus share similar features to a certain extent. However, due to the possible nonlinearity of the implicit constraint, the treatment of the class (IV) is far more difficult. As a consequence of this difficulty, there are no related works on this class as shown in Table 1.

Still, there is a well-known example as a PDE in the class (IV), the (nonlinear) Klein–Gordon (KG) equation in light-cone coordinates

$$(1.10) \qquad u_{tx} = f(u).$$

It is also called "the characteristic form of KG", or "KG in null coordinates." Note that, although there are certainly many studies on the Klein–Gordon equation in *Euclidean coordinates* $u_{\tau\tau} - u_{ss} = f(u)$ (see, e.g., Debnath [10] and references therein), and these two representations are related by the simple transformation $\tau = t + x$, $s = t - x$ of the independent variables, the results on the Euclidean case do not give much useful information for the light-cone case. In fact, if we consider the initial value problem (1.1) for the KG equation in light-cone coordinates, the corresponding problem in Euclidean coordinates is the problem where the "initial data" is given along the line $\tau = -s$, which seems to be aberrant.

Remark 1.1. The nonlinear KG equation in light-cone coordinates has been intensively studied under other boundary conditions. Tuckwell [44] discussed a finite difference scheme under the initial and boundary conditions

$$u(0, x) = \alpha(x) \ (x \in [0, L]), \qquad u(t, 0) = \beta(t) \ (t \in [0, T]),$$

which is introduced by Fokas [13] for the linear KG equation $u_{tx} = u$ and the sine-Gordon equation

$$(1.11) \qquad u_{tx} = \sin u.$$

Recall that, thanks to the presence of the Dirichlet boundary condition, such a case is similar to the case on the whole real line as we described before. Pelloni [35] showed the well-posedness of the sine-Gordon equation with the initial and boundary conditions above. Pellinovsky–Sakovich [34] showed the global well-posedness of the sine-Gordon equation on the whole real line. But, to the best of the

present authors' knowledge, the well-posedness of the sine-Gordon equation (and any other nonlinear KG equation) on the periodic domain has not been developed.

In addition to the above, as we will list in Section 3, various new equations with a mixed derivative have been emerged recently. Therefore, their theoretical and numerical studies are indispensable, and a unified approach to obtain the corresponding integral form that may become their basis is strongly hoped now. However, this has been left open so far, as mentioned before, which might be attributed to the fact that this becomes surprisingly difficult when we proceed from the PDEs in the class (I) toward (IV).

Next, let us illustrate this in more detail. To this end, we discuss to which class Hunter's strategy described before for obtaining the integral form can be applied. First, equations in the class (II) (including (I)) can be transformed into the corresponding integral form in a manner similar to that described before for the reduced Ostrovsky equation.

On the other hand, when one deals with the class (III), the situation is a little bit complicated. In this case, $g(u, u_x, \dots)$ is not a zero-mean function in general, as opposed to the class (II) where $g(u, u_x, \dots) = h_x(u, u_x, \dots)$ is always zero-mean. Thus, the spatial differential operator ∂_x operating on $u_t + g(u, u_x, \dots)$ cannot be regarded as the restricted spatial differential operator $\check{\partial}_x$ (this requires the precise definition including the appropriate regularity of the solution, but here we omit it, and show the rough picture of the difficulty). Still, $u_t(t)$ itself is a zero-mean function so that the equations (1.7) in the class (III) can be rewritten in the separated form

$$\check{\partial}_x u_t + \partial_x g(u, u_x, \dots) = u.$$

Then we follow the same procedure as in the reduced Ostrovsky equation case, except that here we consider the condition that "(a) $u_t \in A$ holds" instead of "(a) $u_t + g \in A$ holds" employed before. Then by using the inverse $\check{\partial}_x^{-1}$, we obtain the integral form

$$u_t + \check{\partial}_x^{-1} \partial_x g(u, u_x, \dots) = \check{\partial}_x^{-1} u.$$

This form has been already pointed out by Miyatake–Yaguchi–Matsuo [31] for the potential Ostrovsky equation (3.6). Although the transformation itself is successful, there remains unusual operator $\check{\partial}_x^{-1} \partial_x$ which does not coincide with the identity operator in general.

Moreover, when it comes to the class (IV), the situation becomes far more challenging. Recall that Hunter's strategy is to "find an exquisite linear subspace A such that (a) $u_t \in A$ holds and (b) $\partial_x|A$ is invertible." Therefore, if we stick to define an inverse of ∂_x for equations in the class (IV), we should consider a (sufficiently small) linear subspace to which u_t belongs. Unfortunately, however, since the solution $u(t)$ is the orbit on $H_f^s(\mathbb{S}) := \{v \in H^s(\mathbb{S}) \mid \mathcal{F}(v) = 0\}$, which is a Banach manifold (see, e.g., [1] for its definition and details) rather than a linear subspace, such a linear subspace should be the tangent space to $H_f^s(\mathbb{S})$ at $u(t)$. Although this can be done for some cases (see, [40]), it involves highly complicated mathematical treatment, and thus we believe it is not a good way to achieve our aim here.

Below, we address our contributions in the present paper. In order to circumvent the difficulty described above, we give up to follow Hunter's strategy, and propose a novel procedure to derive the integral form. There, we employ the Tseng generalized inverse operator ∂_x^{g} (Definition 2.3) of the differential operator ∂_x, which is a standard concept of the generalized inverse for linear operators between Hilbert spaces (see, e.g., [3]). Moreover, we show the equivalence of the differential and integral forms (Theorem 4.9, which corresponds to (A) in Table 1), which has not been explicitly confirmed in the literature. Proposed procedure can be summarized as follows:

(1) Using the property (Lemma 2.7) of generalized inverse operators, we obtain $u_t = g(u, u_x, \dots) + \partial_x^{\mathrm{g}} f(u, u_x, \dots) + c$, where c does not depend on x.

(2) Under some assumptions, by using the implicit constraint $\mathcal{F}(u) = 0$, we determine the value of c by (4.3), and obtain the integral form.

There, the key is that we avoid determining an exquisite linear subspace A in advance. In other words, we give up to directly define an inverse of ∂_x operating on u_t. Instead, we use the Tseng generalized inverse in order to tentatively derive the integral form allowing the unknown constant c, which is then separately determined by using the implicit constraint $\mathcal{F}(u) = 0$.

It should be noted that, the operator $\check{\partial}_x^{-1}$ can be regarded as a special case of the Tseng generalized inverse, so that the reformulation method by Hunter and its followers can be viewed as the special case of our procedure. There, the class of equations such that "Hunter's strategy has been successfully used" can be interpreted as those such that "$c(t) = 0$ thanks to its structure" (see, Example 4.1). Moreover, new procedure gives a more natural way for the class (III) than by the direct use of $\check{\partial}_x^{-1}$ mentioned above (see, Example 4.2).

Remark 1.2. Note that, since the spatial differential operator ∂_x is not invertible, the target equations turn out to be infinite-dimensional DAEs (differential-algebraic equations), whereas the standard evolutionary PDEs are often regarded as infinite-dimensional ODEs (ordinary differential equations). Roughly speaking, proposed procedure can be regarded as an infinite-dimensional extension of the geometric reduction [36] for finite-dimensional DAEs (see, Section 4.2). Since the geometric reduction for DAEs is a basis of unique existence theory for nonlinear DAEs, and all the well-posedness results for equations in the class (I) are based on their integral form, our contribution may be used for PDE-theoretic studies of the PDEs with a mixed derivative. This will be discussed in Section 4.2.

Thanks to the equivalence theorem of the differential and integral forms, there are two ways to devise spatial discretization, i.e., discretizing the differential form or the integral form. It should be noted that the equivalence of the two forms is only valid in continuous case; the discretization of the two forms are essentially different. Section 5 is devoted to discuss this issue (a part of the contents in Section 5 corresponds to (B) in Table 1).

Briefly speaking, the discretization of the integral form becomes an ODE, while the direct spatial discretization of the differential form is an implicit DAE. For such a DAE, in order to derive a corresponding ODE which can be regarded as a discretization of the integral form, the discrete analogue of the proposed procedure above can be used. There, Tseng generalized inverse of the difference operator can be expressed by a generalized matrix of the (matrix expression of) difference operator.

Remark 1.3. The spatial discretization of the differential form can be written in the simple form $D\dot{z} = \phi(z)$, where D is a singular matrix representing a difference operator and $\dot{z} = \mathrm{d}z/\mathrm{d}t$. Its temporal discretization is already discussed in the literature (see, e.g., Hairer–Wanner [18]). Moreover, the obtained DAE often has index one (see, e.g., Ascher–Petzold [2] for details on index of DAEs), and thus, known to be numerically tractable. Therefore, in this paper, we focus on the spatial discretization, and do not step into the temporal discretization.

Though most existing numerical methods have been based on the integral form (see Remark 3.1 for the only known exception), we recommend the *differential form* in practical computation because it

(1) usually has index one;
(2) is free from nonlocal operators (unless g and/or f includes one).

On the other hand, discretization of the integral form has a virtue that it is fit for some analysis.

Finally, we explore the best spatial discretization that should be employed for the mixed derivative (Section 6). There, instead of directly analyzing the difference operator itself, we investigate its generalized inverse as an approximation of the indefinite integral (recall that $\check{\partial}_x^{-1}$ can be regarded as a generalized inverse of ∂_x, which is an indefinite integral). In other words, we compare several discretizations of the differential forms by using their integral forms, which gives an example of the use

of the discretization of the integral form. In the present paper, we take this approach, since it seems, at this moment, there is no systematic way of evaluating discretization errors when PDE involves the mixed derivative.

As a result of this exploration, the average-difference method, which has been recently introduced by the team including present authors [16], turns out to be superior to other standard methods. This fact agrees very well with the numerical observation by Sato–Oguma–Matsuo–Feng [41] for the sine-Gordon equation. Summing up the findings above, we tentatively conclude that, for PDEs with a mixed derivative, the discretization of the differential form with the average-difference method is recommended.

Unfortunately, however, since the average-difference method has been quite recently proposed, it is still less developed. In particular, there are no higher order extensions of the average-difference method, and one may feel that it is not preferable when higher order extensions such as the spectral difference are demanded.

In view of this, as the last contribution of this paper, in order to ease the concern even if only partially, we devise some higher order extensions of the average-difference method and confirm that they surely inherit the good property of the original average-difference method.

The rest of the paper is organized as follows. In Section 2, we show some preliminaries such as function space, variational derivatives, and Tseng generalized inverses. The contents in Sections 3–6 are already described above. Then, the paper is concluded in Section 7.

2. Preliminaries

In this paper, X^s denotes the sth Sobolev space on the periodic domain, i.e., $X^s = H^s(\mathbb{S})$ for a nonnegative integer s, with the standard inner product. Moreover, we define the linear subspace $\check{X}^s$ of X^s as $\check{X}^s := \left\{ v \in X^s \mid \int_{\mathbb{S}} v(x)\mathrm{d}x = 0 \right\}$. If $s \geq 2$, $X^s \subseteq C^1(\mathbb{S})$ holds thanks to the Sobolev inequality so that each element of X^s can be viewed as a continuously differentiable function.

Remark 2.1. We believe that our strategy described in Section 4 can be extended to other settings by appropriately defining the function space (see, Section 7). In order to emphasize that, we here introduce the symbol X^s.

Definition 2.2 (Variational derivatives)**.** For a functional $\mathcal{H} : X^s \to \mathbb{R}$, its variational derivative $\delta\mathcal{H}/\delta v(v)$ is defined as a function such that

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{H}(v + \epsilon\phi)\bigg|_{\epsilon=0} = \left\langle \frac{\delta\mathcal{H}}{\delta v}(v), \phi \right\rangle \qquad (\forall \phi \in X^s)$$

holds, where $\langle \cdot, \cdot \rangle$ is the standard L^2 inner product.

When the funcitonal $\mathcal{H}$ is defined by $\mathcal{H} : v \mapsto \int_{\mathbb{S}} G(v, v^{(1)}, \ldots, v^{(k)})\mathrm{d}x$, its variaitonal derivative can be calculated by

$$\frac{\delta\mathcal{H}}{\delta v}(v) = \sum_{i=0}^{k}(-\partial_x)^i \frac{\partial G}{\partial v^{(i)}}(v, v^{(1)}, \ldots, v^{(k)}),$$

where $v^{(i)}$ is the ith derivative of v for $i \geq 1$ and $v^{(0)} = v$. We often use the abbreviation $\delta\mathcal{H}/\delta v$ for simplicity.

Furthermore, we introduce the generalized inverse of a linear operator between Hilbert spaces (see, e.g., [3]). Here, for a linear operator $L : Y_1 \to Y_2$ between two Hilbert spaces Y_1, Y_2, $\mathrm{dom}(L) \subseteq Y_1$ and $\mathrm{range}(L) \subseteq Y_2$ denote the domain and range of L, respectively. For a closed subspace A of a Hilbert space Y_1, $P_A : Y_1 \to Y_1$ denotes the orthogonal projector on A (i.e., $\mathrm{range}(P_A) = A$ holds).

Definition 2.3 (Tseng generalized inverses)**.** Let $L : Y_1 \to Y_2$ be a linear operator. Then a linear operator $L^{\mathrm{g}} : Y_2 \to Y_1$ is a *Tseng generalized inverse* of L if it satisfies the following four conditions:

$$\mathrm{range}(L) \subseteq \mathrm{dom}(L^{\mathrm{g}}), \qquad\qquad\qquad \mathrm{range}(L^{\mathrm{g}}) \subseteq \mathrm{dom}(L),$$
$$L^{\mathrm{g}} L x = P_{\overline{\mathrm{range}(L^{\mathrm{g}})}} x \quad (x \in \mathrm{dom}(L)), \qquad\qquad L L^{\mathrm{g}} x = P_{\overline{\mathrm{range}(L)}} y \quad (y \in \mathrm{dom}(L^{\mathrm{g}})).$$

Moreover, we introduce the null space $\mathrm{null}(L)$ and the career $\mathrm{car}(L)$ of L, i.e., $\mathrm{null}(L) = \{x \in \mathrm{dom}(L) \mid Lx = 0\}$, $\mathrm{car}(L) = \mathrm{dom}(L) \cap \mathrm{null}(L)^{\perp}$, where $A^{\perp}$ stands for the orthogonal complement of a linear subspace A.

Lemma 2.4 ([3, Chapter 9, Lemma 3])**.** *If L^{g} is a Tseng generalized inverse of L, then* $\mathrm{null}(L) = \mathrm{dom}(L) \cap \mathrm{range}(L^{\mathrm{g}})^{\perp}$ *and* $\mathrm{car}(L) = \mathrm{range}(L^{\mathrm{g}})$ *hold.*

We also define the maximal generalized inverse operator as follows.

Definition 2.5 (Maximal Tseng generalized inverse)**.** Let $L : Y_1 \to Y_2$ be a linear operator. Then, a linear operator $L^{\dagger} : Y_2 \to Y_1$ is called a *maximal Tseng generalized inverse operator* if it is a Tseng generalized inverse operator satisfying $\mathrm{dom}(L^{\dagger}) = Y_2$.

Note that $L^{\mathrm{g}} y = L^{\dagger} y$ holds for any $y \in \mathrm{range}(L)$. This can be checked by using $x \in \mathrm{dom}(L)$ such that $y = Lx$ as follows: $L^{\mathrm{g}} y = L^{\mathrm{g}} L x = L^{\dagger} L x = L^{\dagger} y$. We will use this property in Section 6.

Now, let us introduce Tseng generalized inverse operators of the spatial differential operator $\partial_x : X^s \to X^{s-1}$ (see, e.g., [19, Example 1]). Here, we assume $s \geq 1$. Note that, the differential operator satisfies $\mathrm{dom}(\partial_x) = X^s$, $\mathrm{range}(\partial_x) = \check{X}^{s-1}$, $\mathrm{car}(\partial_x) = \check{X}^s$, and $\mathrm{null}(\partial_x) = \{\alpha \mathbf{1} \in X^s \mid \alpha \in \mathbb{R}\}$. Here, $\mathbf{1}$ denotes a constant function satisfying $\mathbf{1}(x) = 1$ ($x \in \mathbb{S}$). Thus, by Definition 2.3 and Lemma 2.4, each generalized inverse operator ∂_x^{g} satisfies

$$\mathrm{range}(\partial_x) \subseteq \mathrm{dom}(\partial_x^{\mathrm{g}}), \qquad\qquad\qquad \mathrm{range}(\partial_x^{\mathrm{g}}) = \mathrm{car}(\partial_x) = \check{X}^s,$$
$$\partial_x^{\mathrm{g}} \partial_x v = P_{\check{X}^s} v \quad (v \in X^s), \qquad\qquad \partial_x \partial_x^{\mathrm{g}} w = P_{\check{X}^{s-1}} w \quad (w \in \mathrm{dom}(\partial_x^{\mathrm{g}})).$$

It should be noted that, since $\mathrm{dom}(\partial_x^{\mathrm{g}})$ should be a linear subspace of X^{s-1} and $\dim \mathrm{range}(\partial_x)^{\perp} = 1$, $\mathrm{dom}(\partial_x^{\mathrm{g}}) = \check{X}^{s-1}$ or $\mathrm{dom}(\partial_x^{\mathrm{g}}) = X^{s-1}$ hold. This fact implies that there are only two Tseng generalized inverse operators, because the Tseng generalized inverse is uniquely determined by its domain.

The Tseng generalized inverse ∂_x^{g} satisfying $\mathrm{dom}(\partial_x^{\mathrm{g}}) = \mathrm{range}(\partial_x) = \check{X}^{s-1}$ can be concretely expressed as

$$(\partial_x^{\mathrm{g}} v)(x) := \int_0^x v(y) \mathrm{d}y - \frac{1}{2\pi} \int_{\mathbb{S}} \int_0^z v(y) \mathrm{d}y \mathrm{d}z \qquad (v \in \check{X}^{s-1}),$$

which coincides with $\check{\partial}_x^{-1}$ (see, (1.4)) introduced by Hunter [22]. Since $\int_0^x v(y) \mathrm{d}y$ is not periodic if v is not zero-mean, the definition above ceases to work for $v \in X^{s-1} \setminus \check{X}^{s-1}$ so that this operator is not maximal.

On the other hand, the maximal Tseng generalized inverse $\partial_x^{\dagger}$ can be expressed by using the Fourier series as follows:

$$(2.1) \qquad \partial_x^{\dagger} v(x) := \sum_{-\infty < k < \infty,\, k \neq 0} \frac{\hat{v}(k)}{k\mathrm{i}} \exp(k\mathrm{i}x), \qquad\qquad \hat{v}(k) = \frac{1}{2\pi} \int_{\mathbb{S}} v(x) \exp(-k\mathrm{i}x) \, \mathrm{d}x,$$

where i is the imaginary unit. In fact, this operator was already introduced by Yaguchi–Matsuo–Sugihara [46] as an alternative to $\check{\partial}_x^{-1}$. They used $\partial_x^{\dagger}$ in order to describe the pseudospectral method for the Ostrovsky equaiton (3.2) as a discretization of it.

In what follows, we use the symbol $\check{\partial}_x^{-1}$ and $\partial_x^{\dagger}$ when we need to indicate each of the specific Tseng generalized inverses, while ∂_x^{g} is employed when we allow both.

Remark 2.6. Although the concrete examples of Tseng generalized inverses of the spatial differential operator had been used for various equations in the literature (see, Section 3), no one has explicitly described that they can be regarded as a Tseng generalized inverse, to the best of the present authors' knowledge.

The following lemma is an immediate corollary of Lemma 2.4:

Lemma 2.7. *For any $v \in X^s$ and any Tseng generalized inverse operator ∂_x^{g} of ∂_x, there exists a constant $c \in \mathbb{R}$ such that $v(x) = \partial_x^{\mathrm{g}} \partial_x v(x) + c$ holds for any $x \in \mathbb{S}$.*

Proof. By Lemma 2.4 and Definition 2.3, for any $v \in X^s$ it holds that

$$(\partial_x^{\mathrm{g}} \partial_x v)(x) = \left(P_{\overline{\mathrm{range}(\partial_x^{\mathrm{g}})}} v \right)(x) = \left(P_{\check{X}^s} v \right)(x) = v(x) - c \quad (x \in \mathbb{S})$$

for some constant $c \in \mathbb{R}$, which proves the lemma. $\qquad\square$

3. Existing works

In this section, we list equations in each class and existing results on them along Table 1. Unless otherwise stated, existing works below employ $\check{\partial}_x^{-1}$ in order to derive the integral form.

3.1. **Class (I).** The class (I) does not only include the reduced Ostrovsky equation (1.2), but also the short pulse equation [42]

$$(3.1) \qquad \left(u_t - \left(\frac{1}{6} u^3 \right)_x \right)_x = u.$$

It models the propagation of ultrashort optical pulses in nonlinear media.

For any equations in this class, (i) their integral forms can be derived by following the argument for the reduced Ostrovsky equation. For each specific cases, (ii) numerical methods based on their integral forms have been devised in, e.g., [37, 41]. For any equations in this class, (iii) the entropy solution exists uniquely [8] (the local well-posedness has been proved for the short pulse equation [29]). Finally, (iv) Coclite–Ridder–Risebro [8] showed that their numerical method and its convergence analysis can be applicable to any equations in this class. This is the only convergence result for (1.1) that the present authors aware of.

3.2. **Class (II).**

3.2.1. *Ostrovsky equation.* Let us first consider the Ostrovsky equation

$$(3.2) \qquad \left(u_t - \left(\frac{1}{2} u^2 \right)_x + \beta u_{xxx} \right)_x = \gamma u,$$

which has been studied most among various equations in the class (II). It is not in the class (I) unless $\beta = 0$ (i.e., the reduced Ostrovsky equation (1.2)), but is in the class (II), i.e., $f(u) = u$, $h(u, u_x, u_{xx}) = -u^2/2 + \beta u_{xx}$. It originally models the propagation of the gravity waves in a rotating fluid [33]. As its another name, rotation-modified Korteweg–de Vries equation [17], suggests, the case $\gamma = 0$ corresponds to the well-known Koteweg–de Vries equation.

For the Ostrovsky equation (3.2), (i) Yaguchi–Matsuo–Sugihara [46] pointed out that $\check{\partial}_x^{-1}$ and $\partial_x^{\dagger}$ can be used to derive its integral form. (ii) They also devised several finite difference schemes based on its integral form, and Chen–Boyd [6] employed the pseudospectral method. However, to the best of the present authors' knowledge, there are no well-posedness results and mathematical analysis such as convergence analysis for the Ostrovsky equation on $\mathbb{S}$.

It should be noted that there are well-posedness results for the Ostrovsky equation under other boundary conditions (see, e.g., [28]).

3.2.2. *Other equations.* The class (II) does not only include the Ostrovsky equation, but also the Gardner–Ostrovsky equation [20]

$$(3.3) \qquad \left(u_t + cu_x + \alpha \left(u^2\right)_x + \alpha_1 \left(u^3\right)_x + \beta u_{xxx}\right)_x = \gamma u,$$

the generalized Ostrovsky equation [27]

$$(3.4) \qquad \left(u_t + h_x(u) - \beta u_{xxx}\right)_x = \gamma u,$$

where h is a C^2 function which is homogeneous of degree $p \geq 2$, i.e., $vh'(v) = ph(v)$ holds, and the regulalized short pulse equation [9], which is a special case of the generalized Ostrovsky equation with $h(u) = u^3/6$.

For such equations in the class (II), (i) these differential form can be similarly rewritten in the integral form

$$(3.5) \qquad u_t + h_x(u, u_x, \dots) = \check{\partial}_x^{-1} u.$$

We here like to emphasize our point again that, despite some concrete examples in the literature, this general claim itself has not been explicitly written so far. Moreover, (ii) there are several numerical schemes: e.g., Obregon–Stepanyants [32] devised a finite difference scheme for the Gardner–Ostrovsky equation (3.3). However, there are no well-posedness results for them.

3.3. **Class (III).** Miyatake–Yaguchi–Matsuo [31] introduced the potential $\phi = \check{\partial}_x^{-1} u$, and rewrote the Ostrovsky equation as

$$(3.6) \qquad \left(\phi_t - \frac{1}{2}\phi_x^2 + \beta\phi_{xxx}\right)_x = \gamma\phi$$

in order to derive several new structure-preserving methods. In what follows, we call it the potential Ostrovsky equation. Due to the presence of the term ϕ_x^2, this equation cannot be written in the form (1.6), i.e., it is not in the class (II), but is in the class (III).

Although the class (III) is a natural extension of the class (II), currently there are no physical examples except for the potential Ostrovsky equation. Still, this class is introduced in order to clarify the class of equations for which the operator $\check{\partial}_x^{-1}$ effectively works.

As pointed out by Miyatake–Yaguchi–Matsuo [31], (i) the operator $\check{\partial}_x^{-1}$ can operate on both sides of the potential Ostrovsky equation (3.6) as already explained in Introduction. However, the resulting integral form is complicated, and it was not used for numerical computation (see, the remark below). There is no well-posedness result as well.

Remark 3.1. Miyatake–Yaguchi–Matsuo [31] instead proposed various finite difference schemes based on the *differential form*. Since all existing numerical methods for the class (II) ($\supseteq$(I)) are based on their integral form, this is the first numerical method based on the differential form of target PDEs as far as the present authors are aware of.

3.4. **Class (IV).** Most recently, several equations with nonlinear implicit constraints have been emerged. For example, there are the generalized sine-Gordon equation [12]

$$(3.7) \qquad \left(u_t - (\sin u)_x\right)_x = \sin u,$$

the modified Hunter–Saxton equation [11]

$$(3.8) \qquad \left(u_t + \frac{1}{2}\left(u^2\right)_x + \frac{\gamma}{6}u_x^3\right)_x = u + \frac{1}{2}u_x^2,$$

which describes the propagation of short waves in a long wave model, and the modified short pulse equation [39]

$$(3.9) \qquad u_{tx} = u + \frac{1}{2}u\left(u^2\right)_{xx}.$$

Moreover, Tian–Yin [43] proposed another generalization of the Ostrovsky equation whose implicit constraint is nonlinear (see, e.g., [38, 21] for other PDEs in this class).

As of writing the present paper, various studies involving integrability and exact solutions on the whole real line have been conducted one after another. However, the transformation into the integral form has never been discussed, and accordingly there are no related results that requires it (recall Table 1).

4. Transformation between Differential and Integral Forms

In Section 4.1, we propose a new procedure for the transformation of the initial value problem (1.1) into the integral form that gives a unified view for all of (I)–(IV). Then, we show a geometric interpretation of the proposed procedure in Section 4.2. Finally, Section 4.3 is devoted to the equivalence theorem, Theorem 4.9, which summarizes the discussion in this section.

4.1. **Procedure of the Transformation into the Integral Form.** For simplicity, we use the abbreviation such as $f(u)$ which stands for $f(u, u_x, \dots)$ in what follows. Under this abbreviation, we cannot distinguish between the classes (I) and (II), but this will not cause any confusion. We suppose $\mathcal{F}(u_0) = \int_{\mathbb{S}} f(u_0)(x)\mathrm{d}x = 0$ and $s \geq 1$ in this section. Moreover, we assume there exists a solution $u \in C^0([0,T]; X^{s+k}) \cap C^1([0,T]; X^s)$ of the initial value problem (1.1), where k is a nonnegative integer such that $f : X^{s+k} \to X^{s-1}$ and $g : X^{s+k} \to X^s$. Note that, we do not necessarily know whether these assumptions are satisfied in the PDEs (1.1), even in some concrete examples below (recall that well-posedness is proved only for the class (I); see, Table 1). We here emphasize that what we seek here is how we transform them when well-posed, and not the well-posedness itself. It should be noted that, all well-posedness results for the class (I) are proved for their integral forms.

By operating on the both sides of (1.8) with a Tseng generalized inverse operator $\partial_x^{\mathrm{g}} : X^{s-1} \to X^s$, for any $t \in [0,T]$, we see

$$u_t + g(u) = \partial_x^{\mathrm{g}} f(u) + c(t), \tag{4.1}$$

where $c(t)$ does not depend on x from Lemma 2.7. In some happy cases, the implicit constraint $\mathcal{F}(u(t)) = 0$ enables us to determine the value of $c(t)$ as follows.

Since the value of $\mathcal{F}(u(t))$ is always 0 and $u(t)$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(u(t)) = \int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}u_t\mathrm{d}x = \int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}\left(-g(u) + \partial_x^{\mathrm{g}} f(u)\right)\mathrm{d}x + c(t)\int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}\mathrm{d}x, \tag{4.2}$$

the value of $c(t)$ is determined as

$$c(t) = \mathcal{C}(u(t)) := \frac{\int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}\left(g(u) - \partial_x^{\mathrm{g}} f(u)\right)\mathrm{d}x}{\int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}\mathrm{d}x} \tag{4.3}$$

for $t \in [0,T]$ satisfying

$$\int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}\mathrm{d}x \neq 0. \tag{4.4}$$

On the other hand, for $t \in [0,T]$ such that $\int_{\mathbb{S}} \delta\mathcal{F}/\delta u\,\mathrm{d}x = 0$ holds, we obtain a new implicit constraint

$$\mathcal{F}_1(u(t)) = \int_{\mathbb{S}} \frac{\delta\mathcal{F}}{\delta u}\left(g(u) - \partial_x^{\mathrm{g}} f(u)\right)\mathrm{d}x = 0 \tag{4.5}$$

from (4.2), and we can continue the same line of discussion above by using $\mathcal{F}_1$ instead of $\mathcal{F}$.

Fortunately, the most of the examples listed in Section 3 satisfy the condition (4.4) for any $t \in [0,T]$ as we show below. First of all, equations in the class (II) ($\supseteq$ (I)) and (III) obviously satisfy them.

Example 4.1 (Class (II)). The implicit constraint $\mathcal{F}(u) = \int_{\mathbb{S}} u \, \mathrm{d}x = 0$ is linear, and it holds that $\int_{\mathbb{S}} \delta \mathcal{F}/\delta u \, \mathrm{d}x = 2\pi \neq 0$. Therefore, we see

$$\mathcal{C}(u) = \frac{1}{2\pi} \left(\int_{\mathbb{S}} h_x(u) \mathrm{d}x - \int_{\mathbb{S}} \partial_x^{\mathrm{g}} u \, \mathrm{d}x \right) = 0,$$

where the last equality holds by $\mathrm{range}(\partial_x^{\mathrm{g}}) = \check{X}^s$. Thus, it coincides with the transformation by Hunter [22] and its followers if we employ $\mathring{\partial}_x^{-1}$ as the generalized inverse ∂_x^{g}.

Example 4.2 (Class (III)). In this case, the implicit constraint is again linear. However, we see

$$\mathcal{C}(u) := \frac{\int_{\mathbb{S}} \left(g(u) - \partial_x^{\mathrm{g}} u \right) \mathrm{d}x}{2\pi} = \frac{1}{2\pi} \int_{\mathbb{S}} g(u) \mathrm{d}x,$$

and it does not vanish in general. This procedure is quite simple in comparison with the cumbersome argument described in Introduction for deriving the integral form in which we should carefully consider each term is in $\check{X}^{s-1}$ or not. Notice that the new procedure does not cause the unnatural term $\mathring{\partial}_x^{-1} \partial_x g$.

For the class (IV), whether the condition (4.4) holds or not depends on each solution in general.

Example 4.3. If we consider the nonlinear Klein–Gordon equation of the form

$$u_{tx} = u + u^2,$$

we obtain $\delta \mathcal{F}/\delta u = \mathbf{1} + 2u$. Then, the value of $\int_{\mathbb{S}} (\mathbf{1} + 2u) \mathrm{d}x$ depends on time.

Fortunately, the equations listed in Section 3.4 satisfy the condition (4.4) for any $t \in [0, T]$ as follows thanks to some associated conservation laws as far as the initial condition u_0 satisfies $\int_{\mathbb{S}} \delta \mathcal{F}/\delta u(u_0) \, \mathrm{d}x \neq 0$.

Example 4.4 (Sine-Gordon-type equations). For the sine-Gordon equation (1.11) and the generalized sine-Gordon equation (3.7), the implicit constraint $\mathcal{F}(u) = \int_{\mathbb{S}} \sin u \, \mathrm{d}x$ is not linear, and one may feel whether $\int_{\mathbb{S}} \delta \mathcal{F}/\delta u \, \mathrm{d}x = \int_{\mathbb{S}} \cos u \, \mathrm{d}x$ vanishes or not depends on t. But, in fact, $\int_{\mathbb{S}} \cos u \, \mathrm{d}x$ is a conserved quantity of them. Therefore, the value of $c(t)$ can be determined for any $t \in [0, T]$ unless $\int_{\mathbb{S}} \cos u_0(x) \mathrm{d}x = 0$ holds.

Example 4.5 (Modified short pulse equation (3.9)). The implicit constraint

$$\mathcal{F}(u) = \int_{\mathbb{S}} \left(u + \frac{1}{2} u \left(u^2 \right)_{xx} \right) \mathrm{d}x = \int_{\mathbb{S}} \left(u - u u_x^2 \right) \mathrm{d}x$$

is again nonlinear. But in this case, since

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{S}} \frac{1}{2} u_x^2 \mathrm{d}x = \int_{\mathbb{S}} u_x u_{xt} \mathrm{d}x = \int_{\mathbb{S}} u_x \left(u + \frac{1}{2} u \left(u^2 \right)_{xx} \right) \mathrm{d}x = 0$$

and

$$\int_{\mathbb{S}} \frac{\delta \mathcal{F}}{\delta u} \mathrm{d}x = \int_{\mathbb{S}} \left(1 - u_x^2 + (2u u_x)_x \right) \mathrm{d}x = 2\pi - \int_{\mathbb{S}} u_x^2 \mathrm{d}x,$$

the condition (4.4) holds for any $t \in [0, T]$ if $2\pi \neq \int_{\mathbb{S}} \left((u_0)_x \right)^2 \mathrm{d}x$.

We show that the modified Hunter–Saxton equation also satisfies the condition (4.4) later (Example 4.8).

Next, let us consider the cases where the value of $c(t)$ is determined by $\mathcal{F}_1$ instead of $\mathcal{F}$. As of writing this paper, we are not aware of such a physical example, but we can construct an example as follows. (Although this is artificial, we believe this consideration is necessary to set a firm basis for the proposed framework, unless it is proved that such a case never happens in physical applications.)

Example 4.6. For the equation

$$(4.6) \qquad \left(u_t - \frac{1}{2}u^2\right)_x = \frac{1}{2}u_x^2 + \frac{1}{3}u_x^3,$$

the implicit constraint is $\mathcal{F}(u) = \int_{\mathbb{S}}(u_x^2/2 + u_x^3/3)\mathrm{d}x = 0$. Thus, $\int_{\mathbb{S}} \delta\mathcal{F}/\delta u\,\mathrm{d}x = -\int_{\mathbb{S}}\left(u_x + u_x^2\right)_x \mathrm{d}x = 0$ holds for any solution u, and we obtain a new constraint:

$$\mathcal{F}_1(u) = -\int_{\mathbb{S}}\left(u_x + u_x^2\right)_x \left(-\frac{1}{2}u^2 - \partial_x^{\mathrm{g}}\left(\frac{1}{2}u_x^2 + \frac{1}{3}u_x^3\right)\right)\mathrm{d}x$$

$$= -\int_{\mathbb{S}}\left(u_x + u_x^2\right)\left(uu_x + \frac{1}{2}u_x^2 + \frac{1}{3}u_x^3\right)\mathrm{d}x = -\int_{\mathbb{S}}\left(uu_x^2 + uu_x^3 + \varphi(u_x)\right)\mathrm{d}x,$$

where $\varphi(u_x)$ is a polynomial of u_x. Hence, we see

$$\int_{\mathbb{S}}\frac{\delta\mathcal{F}_1}{\delta u}\mathrm{d}x = -\int_{\mathbb{S}}\left(u_x^2 + u_x^3\right)\mathrm{d}x.$$

For such u that this value does not vanish, the value of $c(t)$ can be determined by the (nontrivial) implicit constraint $\mathcal{F}_1(u) = 0$. Otherwise, it reveals that $u_x = 0$ holds for any $x \in \mathbb{S}$ thanks to $\mathcal{F}(u) = 0$, which implies such u is a constant function.

4.2. **Geometric Interpretation of the Proposed Procedure.** This section is devoted to illustrate the intuition of the procedure in the previous section. To this end, we consider its geometric interpretation. Roughly speaking, the proposed procedure can be viewed as the infinite-dimensional version of the "geometric reduction" for finite-dimensional implicit DAEs [36], which gives us the local existence and uniqueness results of them.

However, since the well-posedness of PDEs (1.1) is beyond the scope of this paper, we do not step into the rigorous justification of the infinite-dimensional version of the geometric reduction. Such a justification seems to be challenging, because, for example, the definition of the reducibility itself (see, [36, Definition 4.2]) is only valid for finite-dimensional cases.

First of all, we consider a reduction process for general PDAEs (partial differential-algebraic equations) in the form

$$(4.7) \qquad F(u, u_t) = 0,$$

where $F : X^s \times X^s \to X^s$ is an arbitrary smooth map. When we define the Banach manifold $M = F^{-1}(0)$, the equation (4.7) is equivalent to

$$(4.8) \qquad (u, u_t) \in M.$$

Here, we regard M as a submanifold of TX^s, where TX^s stands for the tangent bundle of X^s. Then, under some appropriate assumptions, the canonical projection $W = \pi(M)$ is a submanifold of X^s ($\pi : TX^s \to X^s$ is a map such that $\pi : (u, v) \mapsto u$). By definition of W, the solution u of the equation (4.7) satisfies $(u, u_t) \in TW$. Then, the solution u of the equation (4.7) also satisfies

$$(4.9) \qquad (u, u_t) \in M_1 := M \cap TW.$$

The process obtaining M_1 from M is called the geometric reduction, and we can further proceed the reduction step such as $W_{i+1} = \pi(M_i)$, $M_{i+1} = TW_{i+1} \cap M_i$ ($i = 1, 2, \dots$).

Now, let us restrict ourselves to the case $F(u, v) := v_x + g_x(u) - f(u)$, i.e., the equation (1.1). In this case, M can be explicitly written in the form

$$M = \{(u, v) \mid \mathcal{F}(u) = 0,\ v = -g(u) + \partial_x^{\mathrm{g}}f(u) + c\mathbf{1}\ (c \in \mathbb{R})\}$$

(recall (4.1)). Then, the canonical projection W of M and its tangent bundle TW can be constructed by

$$W = \pi(M) = \{u \in X \mid \mathcal{F}(u) = 0\},$$

$$TW = \left\{(u, v) \,\bigg|\, \mathcal{F}(u) = 0, \ \frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{F}(u + \epsilon v)\bigg|_{\epsilon=0} = 0\right\}.$$

In a manner similar to that in Section 4.1, M_1 can be written in the form

(4.10)
$$M_1 = \left\{(u, v) \in M \,\bigg|\, \left\langle \frac{\delta\mathcal{F}}{\delta u}, \mathbf{1} \right\rangle \neq 0, \ v = -g(u) + \partial_x^{\mathrm{g}} f(u) + \mathcal{C}(u)\mathbf{1}\right\}$$
$$\cup \left\{(u, v) \in M \,\bigg|\, \left\langle \frac{\delta\mathcal{F}}{\delta u}, \mathbf{1} \right\rangle = 0, \ \mathcal{F}_1(u) = 0\right\}.$$

Here, for $u \in W$ such that $\langle \delta\mathcal{F}/\delta u, \mathbf{1} \rangle \neq 0$, the associated tangent vector v is uniquely determined (namely, the constant c is determined by $\mathcal{C}(u)$, which is defined by (4.3)), while we obtain a new constraint $\mathcal{F}_1(u) = 0$ for $u \in W$ such that $\langle \delta\mathcal{F}/\delta u, \mathbf{1} \rangle = 0$. At every step i, we obtain M_i by a similar reduction process.

When we assume the reduction procedure is successfully well-defined, i.e., the sequence of the Banach manifolds $\{M_i\}_{i=1}^{\infty}$ can be defined, there are three possible scenarios as follows:

(a) $M_i = M_{i+1}$ for some finite positive integer i, and there is *exactly one* tangent vector v such that $(u, v) \in M_i$ for any $u \in \pi(M_i)$:
   In this case, the infinite-dimensional vector field can be uniquely determined. In other words, the equation can be rewritten in the integral form for any initial conditions $u_0 \in \pi(M_i)$.

(b) $M_i = M_{i+1}$ for some finite positive integer i, but this time there are *more than one* tangent vectors v such that $(u, v) \in M_i$ for some $u \in \pi(M_i)$:
   In this case, the result of the reduction process does not provide the integral form at least for some initial conditions.

(c) $M_i \neq M_{i+1}$ holds for any positive integer i:
   This case is the distinctive scenario of the infinite-dimensional case (see, example 4.7 below). We cannot obtain the integral form by the reduction process above.

Below, we show an example which has the infinitely many implicit constraints, i.e., the case (c).

Example 4.7. We consider the following PDE

(4.11)
$$u_{tx} = \frac{1}{3}u_x^3,$$

which is obviously underdetermined since if $u(t, x)$ is a solution, then $u(t, x) + d(t)$ is also a solution for any $d : [0, T] \to \mathbb{R}$ satisfying $d(0) = 0$. Since $\int_{\mathbb{S}} \delta\mathcal{F}/\delta u \, \mathrm{d}x = -\int_{\mathbb{S}}(u_x^2)_x \mathrm{d}x = 0$ holds, we then proceed to obtain a new implicit constraint

$$\mathcal{F}_1(u) = -\int_{\mathbb{S}} \left((u_x^2)_x \, \partial_x^{\mathrm{g}} u_x^2\right) \mathrm{d}x = -\left[(u_x^2) \, \partial_x^{\mathrm{g}} u_x^3\right]_{\mathbb{S}} + \int_{\mathbb{S}} u_x^5 \mathrm{d}x = 3\int_{\mathbb{S}} u_x^5 \mathrm{d}x.$$

In this manner, we can repeat this procedure, and it is easy to verify that at every step i $(i = 1, 2, \dots)$, $\mathcal{F}_i = c_i \int_{\mathbb{S}} u_x^{2i+3} \mathrm{d}x$ holds for some constant c_i. In other words, $M_i \neq M_{i+1}$ holds for any positive integer i.

Note that, when $\langle \delta\mathcal{F}/\delta u, \mathbf{1} \rangle \neq 0$ holds for any $u \in W$, M_1 (defined by (4.10)) can be simply expressed as

$$M_1 = \{(u, v) \mid \mathcal{F}(u) = 0, v = -g(u) + \partial_x^{\mathrm{g}} f(u) + \mathcal{C}(u)\mathbf{1}\},$$

and $M_i = M_1$ holds for any positive integer i. It should be noted that, the discussion on the class (III) $(\supseteq$ (II) $\supseteq$ (I)) in the previous section can be rephrased as this case. However, it is not the case for

the equations in the class (IV) in general. Still, the modified Hunter–Saxton equation, which is in the class (IV), belongs to this case.

Example 4.8. For the modified Hunter–Saxton equation (3.8), the implicit constraint can be expressed as $\mathcal{F}(u) = \int_{\mathbb{S}} \left(u + \frac{1}{2} u_x^2 \right) \mathrm{d}x = 0$. Since

$$\int_{\mathbb{S}} \frac{\delta \mathcal{F}}{\delta u} = \int_{\mathbb{S}} (1 - u_{xx}) \, \mathrm{d}x = 2\pi \neq 0$$

holds for any u, $M_i = M_1$ holds for any i. The integral form can be written in

$$u_t + \frac{1}{2} \left(u^2 \right)_x + \frac{\gamma}{6} u_x^3 = \partial_x^{\mathrm{g}} \left(u + \frac{1}{2} u_x^2 \right) + \mathcal{C}(u),$$

where

$$\mathcal{C}(u) = \frac{1}{2\pi} \int_{\mathbb{S}} (1 - u_{xx}) \left(\frac{1}{2} \left(u^2 \right)_x + \frac{\gamma}{6} u_x^3 - \partial_x^{\mathrm{g}} \left(u + \frac{1}{2} u_x^2 \right) \right) \mathrm{d}x = \frac{\gamma}{12\pi} \int_{\mathbb{S}} u_x^3 \mathrm{d}x.$$

It should be noted that, for such cases as the sine-Gordon equation (i.e., whether the condition (4.4) holds or not depends on the initial condition), M_1 itself does not describe the whole of the vector field. However, if we fix the initial condition u_0 satisfying $\int_{\mathbb{S}} \cos u_0(x) \mathrm{d}x \neq 0$, they can surely be rewritten in the integral form by using one implicit constraint $\mathcal{F}(u) = 0$. This can be done since the procedure in the previous section copes with the single orbit itself, whereas the geometric reduction described in this section is to determine the Banach manifold consisting of all the orbits, and the whole of the vector field on such a manifold.

4.3. **Equivalence of the Two Forms for Smooth Solutions.** We summarize the discussion above in the theorem below. Here, for simplicity, we assume the condition (4.4) holds for any $t \in [0, T]$. Recall that, as shown in Example 4.6, there are equations such that the condition (4.4) does not hold but they can be rewritten in the integral form by our procedure. Still, we here focus on the cases such that (4.4) holds since all physical examples satisfy this assumption.

Theorem 4.9. *Let $f : X^{s+k} \to X^{s-1}$ and $g : X^{s+k} \to X^s$ be mappings for a nonnegative integer k. Suppose that the initial condition u_0 satisfies $\mathcal{F}(u_0) = \int_{\mathbb{S}} f(u_0)(x) \mathrm{d}x = 0$. Then, the solution $u \in C^0([0, T]; X^{s+k}) \cap C^1([0, T]; X^s)$ of the initial value problem (1.1) satisfying $\int_{\mathbb{S}} \delta \mathcal{F}/\delta u \, \mathrm{d}x \neq 0$ ($t \in [0, T]$) is also the solutions of the following initial value problem, and vice versa:*

$$(4.12) \qquad \begin{cases} u_t + g(u) = \partial_x^{\mathrm{g}} f(u) + \mathcal{C}(u) & (t \in [0, T], \ x \in \mathbb{S}), \\ u(0, x) = u_0(x) & (x \in \mathbb{R}). \end{cases}$$

Proof. We already confirmed that the solution $u(t) \in X^s$ of the problem (1.1) is also the solution of the problem (4.12) in Section 4.1. On the other hand, the converse holds since $f(u) \in \check{X}^{s-1}$ holds for any $t \in [0, T]$ thanks to $f(u_0) \in \check{X}^{s-1}$ (recall that $\mathcal{C}(u)$ in (4.12) is constructed in (4.3) so that this claim holds), and $\partial_x \partial_x^{\mathrm{g}}$ is an orthogonal projector on $\check{X}^{s-1}$ (Definition 2.3). $\square$

Note that though the equivalence theorem above strongly relies on the common implicit constraint $\mathcal{F}(u(t)) = 0$, the origins of the constraints in the differential and integral forms are significantly different. In the differential form, the implicit constraint is automatically realized by its structure, namely, the property $\mathbf{1} \in \mathrm{range}(\partial_x)^{\perp}$ of the spatial differential operator ∂_x. On the other hand, in the integral form, the implicit constraint is kept as a nontrivial conserved quantity. This difference has a critical impact over discretization, which is discussed below. Briefly speaking, the former is naturally inherited, while the latter is generally lost unless some explicit care is taken such that it is kept.

5. Classification of Existing Spatial Discretizations and New Variants

Based on the above observation, we consider the finite difference spatial discretization of the initial value problem (1.1). For this purpose, we introduce $u_k : [0, T] \to \mathbb{R}$ ($k \in \mathbb{Z}$) as the approximation of $u(t, k\Delta x)$, where the discrete periodic boundary conditions $u_{k+K} = u_k$ is imposed, and the spatial mesh size Δx is defined as $\Delta x = 2\pi/K$ for some positive integer K. Since we assume the discrete periodicity, we employ the notation $u = (u_1, \dots, u_K)^\top$. Although this is an abuse of symbol, we use this since generally no confusion occurs between this and the continuous solution $u(t, x)$.

In Section 5.1, we compare the discretization of the differential and integral forms. Then, we classify the existing schemes and derive their new variants in Section 5.2.

5.1. **Discretization of the Two Forms.** Here, we point out an extremely important fact that, despite the equivalence theorem in the continuous case, discretizations based on the differential and integral forms can be essentially different.

5.1.1. *Discretization of the integral form.* Since numerical methods for equations in the class (II) had been mainly considered based on the integral form in the literature, let us first start with the integral form. Although existing numerical methods for the class (II) keeps the implicit constraint thanks to its simplicity, when it comes to class (IV), the implicit constraint is violated in general as illustrated below.

Let us for brevity introduce the map $F : X^{s+k} \to X^s$ such that $F(u) = \partial_x^{\mathrm{g}} f(u)$, and consider the discretization

$$(5.1) \qquad \dot{u}_k + \bar{g}_k(u) = \bar{F}_k(u) + \bar{C}(u)$$

of the integral form (4.12), where $\bar{g}_k : \mathbb{R}^K \to \mathbb{R}$ and $\bar{F}_k$ are some approximations of g and F, and $\dot{u}_k$ stands for the time derivative of u_k.

In this case, the equation is an ODE, and generally no constraint is explicitly accompanied here. Thus, unless some special care is taken in the discretization so that a discrete counterpart of the implicit constraint $\mathcal{F}(u) = 0$ successfully results, the solution generally violates the implicit constraint (recall the discussion in the last of the previous section). This is in sharp contrast to the continuous case.

Still, for equations in the class (II), the implicit constraint is linear, and as its consequence, even when we are based on the integral form, we can easily construct a numerical method satisfying a discrete analogue of the linear implicit constraint (see, the examples in the following section).

Another note should go to the fact that, again as opposed to the continuous case, (5.1) cannot be generally reduced to a differential form in the following sense. One may expect that we can obtain a differential form such as

$$\delta_x \dot{u}_k + \delta_x \bar{g}_k = \delta_x \bar{F}_k(u)$$

by some difference operator δ_x such as the forward difference $\delta_x^+ u_k = (u_{k+1} - u_k)/\Delta x$, central difference $\delta_x^{\langle 1 \rangle} u_k = (u_{k+1} - u_{k-1})/(2\Delta x)$, among others. Unfortunately, however, unless the term $\delta_x \bar{F}_k(u)$ can be simplified so that no singular operators appear there, this implicit DAE is obviously underdetermined.

5.1.2. *Discretization of the differential form.* Next, let us consider the direct discretization of the differential form (as described in Remark 3.1, Miyatake–Yaguchi–Matsuo [31] firstly introduced the discretization of the differential form). We show such a discretization keeps a discrete analogue of the implicit constraint so that it can be transformed into another expression, which can be regarded as a discretization of the integral form.

For simplicity, we consider the discretization in the form

$$(5.2) \qquad \delta_x \left(\dot{u}_k + \bar{g}_k(u) \right) = \bar{f}_k(u),$$

where $\bar{f}_k : \mathbb{R}^K \to \mathbb{R}$ is some approximation of f. It should be noted that, the equation (5.2) is a DAE due to the singularity of δ_x (recall Remark 1.3).

Here, we introduce the matrix-vector expression

$$(5.3) \qquad D\left(\dot{u} + \bar{g}(u)\right) = \bar{f}(u),$$

where D is the matrix representation of δ_x, and $\bar{g}$ and $\bar{f}$ are defined as $\bar{g}(u) := (\bar{g}_1(u), \ldots, \bar{g}_K(u))^\top$ and $\bar{f}(u) := (\bar{f}_1(u), \ldots, \bar{f}_K(u))^\top$. We assume D is circulant and $\mathbf{1}^\top D = 0$, where $\mathbf{1} := (1, \ldots, 1)^\top$. These are quite mild assumptions since we impose the discrete periodic boundary condition and employ the uniform grid.

Then, by multiplying $\mathbf{1}^\top$, we see that the solution u of the equation (5.2) automatically satisfies the implicit constraint

$$(5.4) \qquad \mathcal{F}_{\mathrm{d}}(u) := \sum_{k=1}^{K} \bar{f}_k(u)\Delta x = 0 \qquad (\forall t \in [0, T]).$$

Note that, this is a discrete counterpart of the implicit constraint $\mathcal{F}(u) = 0$. Thus, there is a distinct advantage of the differential form.

Furthermore, discretized differential form can be safely transformed to an integral form, which is another advantage. To see this, let us follow the line of the discussion in Section 4.1. By introducing the Tseng generalized inverse δ_x^{g} of a difference operator δ_x, the scheme (5.2) can be transformed into

$$(5.5) \qquad \dot{u}_k + \bar{g}_k(u) = \delta_x^{\mathrm{g}} \bar{f}_k(u) + c(t),$$

where $c(t)$ does not depend on k. It should be noted that, the matrix expression of δ_x^{g} is a generalized inverse matrix of D. In a way similar to the case of the original PDE (Section 4.1), the implicit constraint enables us to determine $c(t)$ under an assumption as follows.

Since the value of $\mathcal{F}_{\mathrm{d}}(u)$ is always 0 and the solution u of the equation (5.5) satisfies

$$(5.6) \qquad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}_{\mathrm{d}}(u) = \nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \dot{u} = \nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \left(-\bar{g}(u) + D^{\mathrm{g}}\bar{f}(u) + c(t)\mathbf{1}\right)$$

('$\cdot$' denotes the standard inner product), the value of $c(t)$ is determined as

$$(5.7) \qquad c(t) = \mathcal{C}_{\mathrm{d}}(u) := \frac{\nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \left(\bar{g}(u) - D^{\mathrm{g}}\bar{f}(u)\right)}{\nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \mathbf{1}}$$

for $t \in [0, T]$ satisfying $\nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \mathbf{1} \neq 0$. Thus, in this case, the equation (5.2) is an implicit DAE with index one (when $\nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \mathbf{1} = 0$, we obtain a new constraint and index is more than one). Under the assumption $\nabla\mathcal{F}_{\mathrm{d}}(u) \cdot \mathbf{1} \neq 0$ $(t \in [0, T])$ (which obviously corresponds to the condition $\int_{\mathbb{S}} \delta\mathcal{F}/\delta u \, \mathrm{d}x \neq 0$), the equation (5.2) is equivalent to

$$(5.8) \qquad \dot{u}_k + \bar{g}_k(u) = \delta_x^{\mathrm{g}} \bar{f}_k(u) + \mathcal{C}_{\mathrm{d}}(u),$$

which can be regarded as a discretization of the integral form (4.12).

Note that, although so far we have considered the simple discretization (5.2), our strategy can easily be applied to other cases. For example, the Ostrovsky equation (3.2) can be rewritten as

$$u_{tx} - u_x^2 - uu_{xx} + \beta u_{xxxx} = \gamma u,$$

whose discretization is not necessarily in the form (5.5). For example, one sometimes should employ the spatial discretization which cannot be written in the form (5.2) in order to maintain the conservation law (see, e.g., (5.15)). Thus, in general, we can consider

$$(5.9) \qquad \delta_x \dot{u}_k + \left(\overline{\partial_x g}\right)_k (u) = \bar{f}_k(u),$$

where $(\overline{\partial_x g})_k$ is an approximation of $\partial_x g$ satisfying $\sum_{k=1}^{K}(\overline{\partial_x g})_k(u) = 0$. Even when we deal with such a case, we can similarly derive the corresponding integral form

$$\dot{u}_k + \delta_x^{\mathrm{g}}\left(\overline{\partial_x g}\right)_k(u) = \delta_x^{\mathrm{g}}\bar{f}_k(u) + \mathcal{C}_{\mathrm{d}}(u), \qquad \mathcal{C}_{\mathrm{d}}(u) = \frac{\nabla\mathcal{F}_{\mathrm{d}}(u)\cdot\left(D^{\mathrm{g}}\left(\overline{\partial_x g}\right)(u) - D^{\mathrm{g}}\bar{f}(u)\right)}{\nabla\mathcal{F}_{\mathrm{d}}(u)\cdot\mathbf{1}}.$$

Although the discretization (5.9) is more general than the simple case (5.2) and includes some practical numerical methods we show below, there is no significant difference between (5.2) and (5.9) in view of the transformation into the integral form. Thus, for simplicity, we employ the simple case in Theorem 5.2, and refer the simple case hereafter.

5.2. **Classification of Existing Methods and Their Equivalents.** In this section, we classify the existing methods (see, Table 2) from the viewpoint of Section 4, and derive their equivalent expressions in another form when possible. Although the full-discretizations are defined in the literature, we show the corresponding semi discretizations by taking the limit $\Delta t \to 0$.

TABLE 2. The classification of the existing methods and their equivalent schemes in another form. Schemes in italic are those newly derived in this paper.

PDE	Differential form (1.1)	Integral form (4.12)
	$u_{tx} + g_x(u) = f(u)$	$u_t + g(u) = F(u) + \mathcal{C}(u)$
Scheme	$\delta_x\dot{u}_k + \delta_x\bar{g}_k(u) = \bar{f}_k(u)$	$\dot{u}_k + \bar{g}_k(u) = \bar{F}_k(u) + \bar{\mathcal{C}}(u)$
	implicit DAE	ODE
Ostrovsky	*average-difference* (5.13)	trapezoidal (5.11)
	Fourier-spectral (5.14)	Fourier-spectral (5.12)
pOstrovsky	central difference (5.15)	*generalized inverse* (5.16)
SG	average-difference (5.17)	*trapezoidal* (5.20)

Yaguchi–Matsuo–Sugihara [46] introduced the discrete counterpart

$$(5.10) \qquad \delta_{\mathrm{FD}}^{-1}u_k = \left(\frac{u_0}{2} + \sum_{i=1}^{k-1}u_i + \frac{u_k}{2}\right)\Delta x - \frac{1}{2\pi}\sum_{i=1}^{K}\left(\frac{u_0}{2} + \sum_{j=1}^{i-1}u_j + \frac{u_i}{2}\right)(\Delta x)^2$$

of $\check{\partial}_x^{-1}$, and devised the norm-preserving scheme

$$(5.11) \qquad \dot{u}_k - \frac{1}{3}\left(\delta_x^{\langle 1\rangle}u_k^2 + u_k\delta_x^{\langle 1\rangle}u_k\right) + \beta\delta_x^{\langle 3\rangle}u_k = \gamma\delta_{\mathrm{FD}}^{-1}u_k$$

for the Ostrovsky equation (3.2). Note that, $\delta_{\mathrm{FD}}^{-1}$ corresponds to the discretization of (1.4) by the trapezoidal rule. Moreover, they devised another norm-preserving scheme

$$(5.12) \qquad \dot{u}_k - \frac{1}{3}\left(\delta_{\mathrm{PS}}u_k^2 + u_k\delta_{\mathrm{PS}}u_k\right) + \beta\delta_{\mathrm{PS}}^3 u_k = \gamma\delta_{\mathrm{PS}}^\dagger u_k$$

by using the Fourier-spectral difference operator δ_{PS} (see, [14] for definition) and its Moore–Penrose pseudoinverse $\delta_{\mathrm{PS}}^\dagger$. Note that, as the notation implies, in the finite-dimensional case, the maximal Tseng generalized inverse coincides with the Moore–Penrose pseudoinverse (see, [3, Chapter 9, Theorem 3]).

These schemes are the discretization of the integral form (4.12), which generally cannot be rewritten in the differential form due to the lack of the implicit constraint. However, the numerical solutions of them satisfies the constraint $\sum_{k=1}^{K}u_k = 0$, which is a discrete counterpart of the implicit constraint of the Ostrovsky equation. This happens since the (original) implicit constraint is linear. Moreover,

the discrete counterparts $\delta_{\mathrm{FD}}^{-1}$ and $\delta_{\mathrm{PS}}^{\dagger}$ of ∂_x^{g} can be regarded as a generalized inverse of some difference operators. Thus, they have corresponding expression in the differential form (1.1): in fact, the trapezoidal scheme (5.10) can be equivalently rewritten as

$$(5.13) \qquad \delta_x^+ \left(\dot{u}_k - \frac{1}{3} \left(\delta_x^{\langle 1 \rangle} u_k^2 + u_k \delta_x^{\langle 1 \rangle} u_k \right) + \beta \delta_x^{\langle 3 \rangle} u_k \right) = \gamma \mu_x^+ u_k,$$

where the forward average operator μ_x^+ is defined as $\mu_x^+ u_k = (u_k + u_{k+1})/2$, and the Fourier-spectral scheme (5.12) can be equivalently rewritten as

$$(5.14) \qquad \delta_{\mathrm{PS}} \left(\dot{u}_k - \frac{1}{3} \left(\delta_{\mathrm{PS}} u_k^2 + u_k \delta_{\mathrm{PS}} u_k \right) + \beta \delta_{\mathrm{PS}}^3 u_k \right) = \gamma u_k.$$

Miyatake–Yaguchi–Matsuo [31] devised the norm-preserving scheme

$$(5.15) \qquad \delta_x^{\langle 1 \rangle} \dot{\phi}_k - \frac{1}{3} \left(\left(\delta_x^{\langle 1 \rangle} \phi_k \right) \delta_x^{\langle 1 \rangle} + \delta_x^{\langle 1 \rangle} \left(\delta_x^{\langle 1 \rangle} \phi_k \right) \right) \left(\delta_x^{\langle 1 \rangle} \phi_k \right) + \beta \delta_x^{\langle 4 \rangle} \phi_k = \gamma \phi_k$$

for the potential Ostrovskey equation (3.6), which is in differential form. Since the assumption $\nabla \mathcal{F}_{\mathrm{d}}(u) \cdot \mathbf{1} \neq 0$ always holds thanks to the linear implicit constraint, it can be transformed into the integral form

$$(5.16) \qquad \dot{\phi}_k - \frac{1}{3} \left(\delta_x^{\langle 1 \rangle} \right)^{\dagger} \left(\left(\delta_x^{\langle 1 \rangle} \phi_k \right) \delta_x^{\langle 1 \rangle} + \delta_x^{\langle 1 \rangle} \left(\delta_x^{\langle 1 \rangle} \phi_k \right) \right) \left(\delta_x^{\langle 1 \rangle} \phi_k \right) + \beta \left(\delta_x^{\langle 1 \rangle} \right)^{\dagger} \delta_x^{\langle 4 \rangle} \phi_k$$
$$= \gamma \left(\delta_x^{\langle 1 \rangle} \right)^{\dagger} \phi_k.$$

In the transformations of the schemes (5.12) and (5.15), the Moore–Penrose pseudoinverse is used as one of the generalized inverses. On the other hand, in the transformation of the scheme (5.11) into (5.13), the summation by the trapezoidal rule is used as one of the generalized inverses of the average-difference (δ_x^+, μ_x^+), which is recently devised by Furihata–Sato–Matsuo [16]. It can be generalized as shown in the theorem below.

Remark 5.1. Strictly speaking, since the average-difference had not been rigorously defined as a linear operator (see, Remark 6.1), its generalized inverse can not be defined too at this moment. However, as shown in the theorem below, the operator $\delta_{\mathrm{FD}}^{-1}$ can be used like as the generalized inverse of the average-difference.

Moreover, the team including present authors has already obtained some results on this issue (see, Section 7). In fact, the average-difference can be defined as a linear operator, and there actually $\delta_{\mathrm{FD}}^{-1}$ can be regarded as its Tseng generalized inverse. Due to the restriction of the space and since this topic is beyond the scope of this paper, we do not step into such a justification here.

Theorem 5.2. *Suppose that the initial condition $(u_k(0) \mid k = 1, \ldots, K)$ satisfies $\sum_{k=1}^{K} \bar{f}_k(u(0)) = 0$, and $\sum_{j=1}^{K} \sum_{k=1}^{K} \frac{\partial \bar{f}_j}{\partial u_k}(u(t)) \neq 0$ holds for any $t \in [0, T]$. Then, the average-difference method*

$$(5.17) \qquad \delta_x^+ \left(\dot{u}_k + \bar{g}_k(u) \right) = \mu_x^+ \bar{f}_k(u)$$

is equivalent to

$$(5.18) \qquad \dot{u}_k + \bar{g}_k(u) = \delta_{\mathrm{FD}}^{-1} \bar{f}_k(u) + \mathcal{C}_{\mathrm{d}}(u),$$

where $\mathcal{C}_{\mathrm{d}}(u)$ is defined as

$$\mathcal{C}_{\mathrm{d}}(u) = \frac{\sum_{j=1}^{K} \sum_{k=1}^{K} \frac{\partial \bar{f}_j}{\partial u_k}(u) \left(\bar{g}_k(u) - \delta_{\mathrm{FD}}^{-1} \bar{f}_k(u) \right)}{\sum_{j=1}^{K} \sum_{k=1}^{K} \frac{\partial \bar{f}_j}{\partial u_k}(u)}.$$

Proof. First, we derive the integral form (5.18) from the differential form (5.17). By summing the both sides of (5.17) for $k = 1, \ldots, j - 1$, we see

$$\frac{\dot{u}_j - \dot{u}_1}{\Delta x} + \frac{\bar{g}_j(u) - \bar{g}_1(u)}{\Delta x} = \frac{\bar{f}_0(u)}{2} + \sum_{k=1}^{j-1} \bar{f}_k(u) + \frac{\bar{f}_j}{2},$$

which is equivalent to

$$\dot{u}_k + \bar{g}_k(u) = \delta_{\mathrm{FD}}^{-1} \bar{f}_k(u) + c(t),$$

where $c(t)$ does not depend on k. Note that, the equation above corresponds to (4.1). Therefore, analogously, in order to determine the value of $c(t)$, we can use the implicit constraint $\sum_{k=1}^{K} \mu_x^+ \bar{f}_k(u) = 0$, which is satisfied for any solutions of (5.17). Before following the argument (4.2), notice that, thanks to the discrete periodicity, $\sum_{k=1}^{K} \mu_x^+ \bar{f}_k(u) = \sum_{k=1}^{K} \bar{f}_k(u)$ holds, which allows us to use the simple constraint $\sum_{k=1}^{K} \bar{f}_k(u) = 0$. Then, we see

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} \sum_{k=1}^{K} \bar{f}_k(u) = \sum_{j=1}^{K} \sum_{k=1}^{K} \frac{\partial \bar{f}_k}{\partial u_j}(u) \dot{u}_j = \sum_{j=1}^{K} \sum_{k=1}^{K} \frac{\partial \bar{f}_k}{\partial u_j}(u) \left(-\bar{g}_k(u) + \delta_{\mathrm{FD}}^{-1} \bar{f}_j(u) + c(t) \right)$$

Thus, we obtain $c(t) = \mathcal{C}_{\mathrm{d}}(u)$ under the assumption of the theorem.

Now, let us prove the converse. Note that, for any zero-mean vector v (i.e., $\sum_{k=1}^{K} v_k = 0$ holds), $\delta_x^+ \delta_{\mathrm{FD}}^{-1} v_k = \mu_x^+ v_k$ is satisfied (this claim can be verified by simple calculation). Therefore, the solution u of (5.18) also satisfies (5.17) due to $\sum_{k=1}^{K} \bar{f}_k(u) = 0$, which is kept by the definition of $\mathcal{C}_{\mathrm{d}}$. ☐

By using the theorem above, we see that the average-difference method [41]

(5.19) $$\delta_x^+ \dot{u}_k = \mu_x^+ \sin u_k$$

for the sine-Gordon equation (1.11) is equivalent to

(5.20) $$\dot{u}_k = \delta_{\mathrm{FD}}^{-1} \sin u_k - \frac{\sum_{k=1}^{K} \cos u_k \delta_{\mathrm{FD}}^{-1} \sin u_k}{\sum_{k=1}^{K} \cos u_k},$$

unless $\sum_{k=1}^{K} \cos u_k = 0$. This assumption, however, can be replaced by that for the initial condition, because $\sum_{k=1}^{K} \cos u_k$ is a conserved quantity of the average-difference method (5.19) (see, [16, Theorem 1]). As can be seen, the integral form (5.20) has nonlocal operator $\delta_{\mathrm{FD}}^{-1}$ and thus in this sense (5.20) is more complicated than (5.19).

Summing up all the observations, let us close this section with the summary below. In general, the discretizations of differential and integral forms have the following features, respectively:

- Discretizations of the differential form
    - \+ are often free from nonlocal operator;
    - \+ automatically have an implicit constraint corresponding to $\mathcal{F}(u) = 0$;
    - − are implicit DAEs (but usually has index one);
    - \+ can be almost always rewritten in the integral form.
- Discretizations of the integral form
    - − must have nonlocal operator;
    - − can lose the implicit constraint;
    - \+ are merely ODEs;
    - − cannot be rewritten in the differential form in general.

Counting all the above pros and cons, we believe that, for actual computation, the discretization of the differential form should be employed. For the third points, in particular, it should be noted that a reduction to an ODE is known to be unpractical for the large DAE representing an electrical network involving a large and sparse matrix, because the sparsity is destroyed by the reduction (see, e.g. [2, Example 9.3]). Since the spatial discretization of the differential form also involves a large and sparse matrix, we believe it should be numerically treated as is, namely, without a reduction to an ODE.

On the other hand, the discretization of the integral form may fit to analyzing the property of the scheme as we will show an example in Section 6, where we have more intense look at the discretization of the differential form.

6. On Spatial Discretization of the Mixed Derivative

In this section, we discuss which difference operators are suitable for the spatial discretization of the mixed derivative. Since the method of some mathematical analysis on numerical schemes in the form (5.2) is yet to be investigated as mentioned in Introduction, we prefer to be based on another expression (5.8), which is just an ODE. We first investigate the accuracy of generalized inverse δ_x^{g} of each difference operator δ_x in Section 6.1. This is sufficient because the emergence of δ_x^{g} is the only distinct property of (5.8). As a result, we conclude that the average-difference is the best way to discretize the mixed derivative among 2nd order differences. This consequence agrees very well with the numerical observation for some specific cases [41, 16]. Then, in Section 6.2, we newly introduce some higher order extensions of the average-difference method, and confirm they inherit the good property of the average-difference method.

6.1. **Analysis of the Generalized Inverses of Difference Operators.** Since the difference operator δ_x is an approximation of the differential operator ∂_x, one may expect that δ_x^{g} is also an approximation of ∂_x^{g}. Notice also that it is enough to just consider $\mathring{\partial}_x^{-1}$ as ∂_x^{g}, since in (4.12) ∂_x^{g} is only applied to zero-mean functions, and as noted after Definition 2.5 $\partial_x^{\mathrm{g}} v = \partial_x^\dagger v$ holds for such functions. Thus, we expect the relation

$$(6.1) \qquad \delta_x^{\mathrm{g}} v_k - \delta_x^{\mathrm{g}} v_{k-1} \approx \int_{(k-1)\Delta x}^{k\Delta x} v(y)\mathrm{d}y.$$

for $v : \mathbb{S} \to \mathbb{R}$ and $v_k \approx v(k\Delta x)$. Here, we assume $(v_k \mid k = 1, \ldots, K) \in \mathrm{range}(\delta_x)$, since δ_x^{g} is usually applied to such vectors (see, Section 5.1.2). Thanks to $\mathrm{range}(\delta_x) \subseteq \mathrm{dom}(\delta_x^{\mathrm{g}})$, this assumption justifies that δ_x^{g} can be applied to v_k. Moreover, again as noted after Definition 2.5, this assumption implies $\delta_x^{\mathrm{g}} v_k = \delta_x^\dagger v_k$ holds, i.e., the values of $\delta_x^{\mathrm{g}} v_k$ are the same for any Tseng inverses.

In order to verify the accuracy of the approximation in (6.1), let us consider $u^\omega(x) = \exp(\mathrm{i}\omega x)$ ($\omega \in \mathbb{Z}$), i.e., each frequency component of the Fourier series. Then, the exact value $I_k(\omega)$ of the integration on $[(k-1)\Delta x, k\Delta x]$ can be computed as

$$(6.2) \qquad I_k(\omega) := \int_{(k-1)\Delta x}^{k\Delta x} \exp(\mathrm{i}\omega x)\mathrm{d}x = \frac{2}{\omega} \exp\left(\mathrm{i}\omega\left(k - \frac{1}{2}\right)\Delta x\right) \sin\frac{\omega\Delta x}{2}.$$

Now, let us consider the approximation $\bar{I}_k(\omega) := \delta_x^{\mathrm{g}} u_k^\omega - \delta_x^{\mathrm{g}} u_{k-1}^\omega$ of I_k, where $u_k^\omega := u^\omega(k\Delta x) = \exp(\mathrm{i}\omega k\Delta x)$. In what follows, we only use the notation u_k^ω as a single component (i.e., u_k^ω denotes a scholar, and u^ω denotes a function itself) in order to avoid the ambiguity of possible confusions between the continuous function and the vectors (in Section 5). Notice that, for any $\omega \in \mathbb{Z}$, the vector $(u_k^\omega \mid k = 1, \ldots, K)$ is one of the eigenvectors of the matrix representation D of δ_x, because D is assumed to be circulant. Namely, $\delta_x u_k^\omega = \lambda_\omega u_k^\omega$ holds for any $\omega \in \mathbb{Z}$ and $k \in \mathbb{Z}$, where λ_ω is the corresponding eigenvalue, and $\lambda_{\omega+K} = \lambda_\omega$ holds for any $\omega \in \mathbb{Z}$. Then, since $\delta_x^{\mathrm{g}} v = \delta_x^\dagger v$ holds

for any $v \in \mathrm{range}(\delta_x)$ (recall the discussion immediately after Definition 2.5) and the Moore–Penrose pseudoinverse $D^\dagger$ of the circulant matrix D is also circulant, we see

$$\delta_x^{\mathrm{g}} u_k^\omega = \delta_x^\dagger u_k^\omega = \lambda_\omega^{-1} u_k^\omega = \lambda_\omega^{-1} \exp(\mathrm{i}\omega k \Delta x)$$

for $\omega \in \{n \in \mathbb{Z} \mid \lambda_n \neq 0\}$ (recall $\mathrm{dom}(\check{\partial}_x^{-1}) = \check{X}^{s-1} = \mathrm{range}(\partial_x)$, and notice $(u_k^\omega \mid k = 1, \ldots, K) \in \mathrm{range}(\delta_x) \iff \lambda_\omega \neq 0$). Therefore, for such ω, it holds that

$$(6.3) \qquad \bar{I}_k(\omega) := \delta_x^{\mathrm{g}} u_k^\omega - \delta_x^{\mathrm{g}} u_{k-1}^\omega = 2\mathrm{i}\lambda_\omega^{-1} \exp\left(\mathrm{i}\omega \left(k - \frac{1}{2} \right) \Delta x \right) \sin \frac{\omega \Delta x}{2}.$$

By combining (6.2) and (6.3), we see $\bar{I}_k(\omega) = \mathrm{i}\lambda_\omega^{-1}\omega I_k(\omega)$. Furthermore, we can easily compute the relative error $e(\tilde{\omega})$ as follows:

$$(6.4) \qquad e(\tilde{\omega}) := \left| \frac{\bar{I}_k(\omega) - I_k(\omega)}{I_k(\omega)} \right| = \left| \mathrm{i}\lambda_\omega^{-1}\omega - 1 \right|,$$

where $\tilde{\omega} = \omega \Delta x$ is the scaled wave number.

Note that, there are the implicitly defined finite differences such as the average-difference and the compact difference (see, e.g., [26]), i.e., $U_x = u$ is discretized as $\delta_x U_k = \mu_x u_k$ with the pair of a difference operator δ_x and an average operator μ_x. For example, the average-difference is defined by $\delta_x^+ U_k = \mu_x^+ u_k$, and the compact difference is defined by $\delta_x^{a,b,c} U_k = \mu_x^{\alpha,\beta} u_k$, where

$$\delta_x^{a,b,c} U_k = \frac{2cU_{k+3} + 3bU_{k+2} + 6aU_{k+1} - 6aU_{k-1} - 3bU_{k-2} - 2cU_{k-3}}{12\Delta x},$$
$$\mu_x^{\alpha,\beta} u_k = \beta u_{k+2} + \alpha u_{k+1} + u_k + \alpha u_{k-1} + \beta u_{k-2}$$

and α, β, a, b, c are parameters. Even in these cases, similar argument can be done by using the eigenvalues of $D^\dagger M$ instead of λ_ω^{-1}'s, where D and M are the matrix representations of δ_x and μ_x.

Remark 6.1. The compact difference operators are well-defined thanks to the diagonal dominance of the matrix M. On the other hand, since M is singular if K is even for the average-difference, its definition as a linear operator itself is challenging. In this paper, we do not step into this issue as we described in Remark 5.1.

Therefore, the order of the average-difference cannot be defined in usual sense. However, we compare it with 2nd order difference operators since the average-difference reproduce the exact value up to 2nd order polynomials, which is a common feature of 2nd order difference operators (see, e.g., Fornberg [14]).

The relative errors $e_{\mathrm{CD2}}(\tilde{\omega})$, $e_{\mathrm{OD2}}(\tilde{\omega})$, and $e_{\mathrm{AD2}}(\tilde{\omega})$ of the 2nd order central difference, 2nd order one-sided difference $(-u_{k+2} + 4u_{k+1} - 3u_k)/(2\Delta x)$, and average-difference can be computed as

$$e_{\mathrm{CD2}}(\tilde{\omega}) = \left| \frac{\tilde{\omega}}{\sin \tilde{\omega}} - 1 \right|, \qquad\qquad e_{\mathrm{OD2}}(\tilde{\omega}) = \left| \frac{2\mathrm{i}\tilde{\omega}}{-3 + 4\exp(\mathrm{i}\tilde{\omega}) - \exp(2\mathrm{i}\tilde{\omega})} - 1 \right|$$
$$e_{\mathrm{AD}}(\tilde{\omega}) = \left| \frac{\tilde{\omega}}{2\tan(\tilde{\omega}/2)} - 1 \right|$$

for $\tilde{\omega} \notin \{n\pi \mid n \in \mathbb{Z}\}$. On the other hand, the relative error $e_{\mathrm{PS}}(\tilde{\omega})$ for $\tilde{\omega} \notin \{n\pi \mid n \in \mathbb{Z}\}$ of the Fourier-spectral difference is

$$e_{\mathrm{PS}}(\omega) = \begin{cases} |2n\pi/(\tilde{\omega} - 2n\pi)| & (\tilde{\omega} \in (2n\pi, 2(n+1)\pi)) \\ |2(n+1)\pi/((2n+1)\pi - \tilde{\omega})| & (\tilde{\omega} \in ((2n+1)\pi, (2n+2)\pi)) \end{cases}.$$
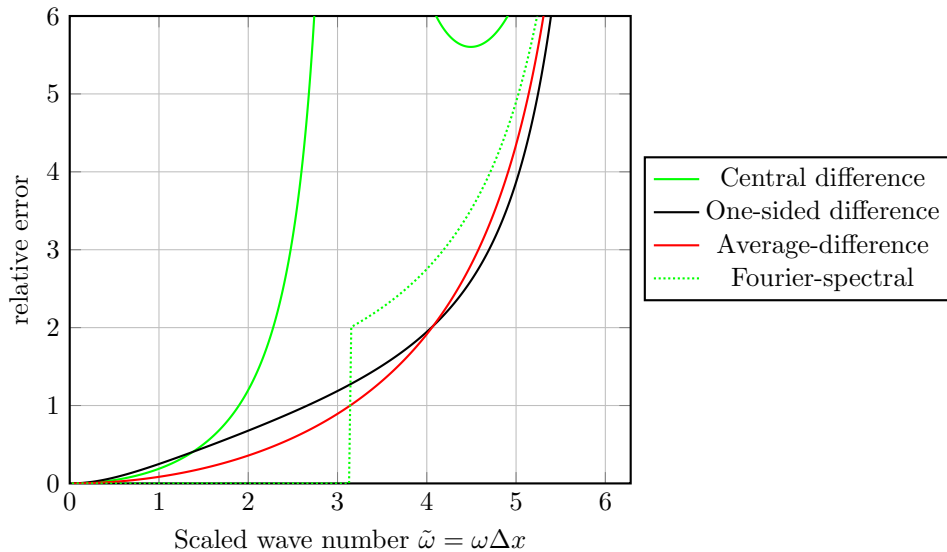
These relative errors are summarized in Figure 1.

FIGURE 1. The relative errors $e(\tilde{\omega})$ of 2nd order difference operators and the Frourier-spectral difference operator.

Figure 1 shows that the average-difference is far better than the central difference, in particular, for high frequency components. This fact is in good agreement with the observation by Sato–Oguma–Matsuo–Feng [41] for the sine-Gordon equation (see, [41, Fig.14 and 16]). There, numerical solutions obtained by a finite difference method with the central difference strongly suffer from artificial oscillation, while those by the average-difference method reproduce the solution very well. Moreover, for frequency components above the Nyquist frequency $\tilde{\omega} = \pi$, the average-difference is superior to the Fourier-spectral difference. This agrees well with the observation by Furihata–Sato–Matsuo [16] for the linear Klein–Gordon equation with the square wave (see, [16, Fig. 3]). There, numerical solutions obtained by the central difference, Fourier-spectral difference, and average-difference are compared, and it was found that those by the central and Fourier-spectral differences suffer from artificial oscillation, while again, the average-difference reproduces better numerical solutions.

The behavior of the one-sided difference is similar to that of the average-difference method. However, the average-difference method is better than the one-sided difference for most frequency components.

As a result, we conclude that the average-difference method is the best among the 2nd order difference methods considered here. It should be noted that, the target initial value problem in the form (1.1) involves equations whose solutions tend to have steep fronts (see, e.g., [29, 30]). Therefore, the behavior of high-frequency component is often important, and the conclusion here is expected to extend to wide range of PDEs (1.1). In what follows, we compare methods from this standpoint.

However, the average-difference method has been recently devised and thus less investigated. For example, its higher order extensions have not been discussed whereas higher order one-sided difference, central difference, and compact difference operators are well developed. This might give an impression that the direction this paper suggests, i.e., the use of the average-difference method is not necessarily promising. To partially ease this concern, in the next section, we consider an extension of the average-difference method.

Remark 6.2. The average-difference method resembles the box scheme. In fact, the average-difference method for the advection equation $u_t = u_x$ coincides with the box scheme (detailed analysis on the box

scheme and its higher order extensions for the advection equation can be found in Frank–Reich [15]). Therefore, the average-difference method also resembles to multisymplectic integrators (see, e.g., [25]). For example, the Preissman box scheme for the linear Klein–Gordon equation $u_{tx} = u$ coincides with the average-difference method with the implicit midpoint rule for temporal discretization.

However, the direction of the extension to nonlinear case and their scope are different. The average-difference method was investigated in Furihata–Sato–Matsuo [16] with special emphasis on its application to the equations in the form $u_{tx} = \delta\mathcal{H}/\delta u$, while the Preissman box scheme is designed for maintaining the discrete multisymplecticity.

6.2. **Extension of the Average-Difference Method.** In this section, we consider a higher order extension of the average-difference method. However, directly extending it seems to be difficult because there are many possibilities. Therefore, in view of the relation $\delta_x^+ \delta_{\text{FD}}^{-1} v_k = \mu_x^+ v_k$ ($(v_k \mid k = 1, \dots, K)$ is a zero-mean vector) connecting the average-difference method (δ_x^+, μ_x^+) and the trapezoidal rule δ_{FD}^{-1}, we first consider a higher order extension $\delta_{\text{FD},s}^{-1}$ of the trapezoidal rule instead of that of the average-difference method. Then, we define the extended average-difference method $(\delta_x^+, \mu_x^{+,s})$ by introducing the extended forward average operator $\mu_x^{+,s}$ such that $\mu_x^{+,s} v_k = \delta_x^+ \delta_{\text{FD},s}^{-1} v_k$ holds for any zero-mean vector $(v_k \mid k = 1, \dots, K)$.

To this end, let us first consider a higher order extension of the trapezoidal rule for the indefinite integral. Recall that the trapezoidal discretization (5.10) uses the approximation such as

$$(6.5) \qquad \frac{v_1 + v_0}{2}\Delta x \approx \int_0^{\Delta x} v(y)\mathrm{d}x$$

for each interval $[(k-1)\Delta x, k\Delta x]$, where $v_k := v(k\Delta x)$. The left-had side can be regarded as the exact integration of the linear interpolation of $((k-1)\Delta x, v_{k-1})$ and $(k\Delta x, v_k)$. In order to finally derive the extended average operator $\mu_x^{+,s}$ such that locally defined, we should carefully extend the trapezoidal rule here. In fact, it can be done by using the Lagrange interpolation as follows.

Here, we consider the $(2s-1)$th order Lagrange interpolation

$$p^{(s)}(x) = \sum_{j=-s+1}^{s} v_j l_j^{(s)}(x), \qquad\qquad l_j^{(s)}(x) = \frac{\prod_{-s+1\le i\le s;\ i\ne j}(x - i\Delta x)}{\prod_{-s+1\le i\le s;\ i\ne j}(j - i)\Delta x},$$

where we use $2s$ nodes $(-s+1)\Delta x, (-s+2)\Delta x, \dots, 0, \Delta x, \dots, (s-1)\Delta x, s\Delta x$ for the interpolation. Then, by using $p^{(s)}$, we can approximate the right-hand side of (6.5):

$$\int_0^{\Delta x} v(y)\mathrm{d}x \approx \int_0^{\Delta x} p^{(s)}(x)\mathrm{d}x = \sum_{i=-s+1}^{s} v_j \int_0^{\Delta x} l_j^{(s)}(x)\mathrm{d}x.$$

Note that it coincides with the trapezoidal rule when $s = 1$. Since $\int_0^{\Delta x} l_j^s(x)\mathrm{d}x = \int_0^{\Delta x} l_{-j+1}^s(x)\mathrm{d}x$ holds for any $j > 0$, the approximation above can be simplified into

$$(6.6) \qquad \int_0^{\Delta x} v(y)\mathrm{d}x \approx \sum_{j=1}^{s} \mu_j^{(s)} \left(v_j + v_{1-j}\right)\Delta x$$

for any positive integer s, where $\mu_j^{(s)} = (1/\Delta x)\int_0^{\Delta x} l_j^{(s)}(x)\mathrm{d}x$. For example, it holds that

$$\mu_1^{(1)} = \frac{1}{2},$$

$$\mu_1^{(2)} = \frac{13}{24}, \qquad\qquad \mu_2^{(2)} = -\frac{1}{24},$$

$$\mu_1^{(3)} = \frac{401}{720}, \qquad\qquad \mu_2^{(3)} = -\frac{31}{480}, \qquad\qquad \mu_3^{(3)} = \frac{11}{1440}.$$

By using the $(2s-1)$th order approximation (6.6), we can define an extension $\delta_{\mathrm{FD},s}^{-1}$ as follows:

$$\delta_{\mathrm{FD},s}^{-1} v_k = \sum_{j=1}^{k} \left(\sum_{i=1}^{s} \mu_i^{(s)} (v_{j+i} + v_{j+1-i}) \Delta x \right) - \frac{1}{K} \sum_{j=1}^{K} \left(\sum_{i=1}^{s} \mu_i^{(s)} (v_{j+i} + v_{j+1-i}) \Delta x \right),$$

where $\delta_{\mathrm{FD},1}^{-1} = \delta_{\mathrm{FD}}^{-1}$ holds. It should be noted that, by definition, $\delta_{\mathrm{FD},s}^{-1}$ reproduce the exact value up to $(2s-1)$th order polynomial.

Now, let us define an extension of the average-difference method $(\delta_x^+, \mu_x^{+,s})$ by using the relation $\mu_x^{+,s} v_k = \delta_x^+ \delta_{\mathrm{FD},s}^{-1} v_k$. Here, the extended average operators $\mu_x^{+,s}$ turn out to be expressed as

$$\mu_x^{+,s} v_k := \sum_{j=1}^{s} \mu_j^{(s)} \left(v_{k+j} + v_{k+1-j} \right).$$

For example, $\mu_x^{+,2}$ and $\mu_x^{+,3}$ can be written as

$$\mu_x^{+,2} v_k := \frac{-v_{k-1} + 13v_k + 13v_{k+1} - v_{k+2}}{24},$$
$$\mu_x^{+,3} v_k := \frac{11v_{k-2} - 93v_{k-1} + 802v_k + 802v_{k+1} - 93v_{k+2} + 11v_{k+3}}{1440}.$$

It should be noted that, since $\delta_{\mathrm{FD},s}^{-1}$ reproduces the exact value up to $(2s-1)$th order polynomials, the extended average-difference $(\delta_x^+, \mu_x^{+,s})$ reproduces the exact value up to $2s$th order polynomials.

The relative error $e(\tilde{\omega})$ corresponds to these extensions of the average-difference method can be similarly computed. They are compared with several difference operators such as various compact differences in Figure 2 (see, e.g., [24, 14] for the definitions of each difference operator). Similar to the original average-difference (recall, Remark 6.1), whether these extensions can be regarded as the difference operators is unclear. Thus, again, the order of them cannot be defined in the usual sense. However, since they reproduce the exact value up to $2s$th polynomials as we described above, we compare them with $2s$th order difference operators.

As shown in Figure 2, the average-difference-type methods (AD2–AD6) are again far better than central differences (CD2–CD6). Tridiagonal compact differences (TC4, TC6) are slightly better than the average-differences for low frequency components, but again, the opposite happens for high frequency components.

Spectral-like compact difference (SLC6) is better than the others except for the Fourier-spectral difference in $\tilde{\omega} < 2.8$. However, it is far worse than the average-difference method around the Nyquist frequency. In view of this, a spectral-like extension of the average-difference method seems worth investigation (see, Section 7).

Since the coefficients of the one-sided differences diverge when its order becomes higher, its relative error does not converge to that of the Fourier-spectral difference operator. In fact, when $p \to \infty$, the relative error $e_{\mathrm{OD}p}(\tilde{\omega})$ of pth order one-sided difference operator converges to 0 if $\tilde{\omega} \in (0, \pi/3)$, and 1 if $\tilde{\omega} \in (\pi/3, \pi)$. Though the relative errors of one-sided differences near the Nyquist frequency is acceptable, that of around $\tilde{\omega} = \pi/2$ is far worse than the other differences. In view of this, we conclude one-sided differences should not be employed for discretizing the mixed derivative.

Therefore, the extensions of the average-difference method are expected to be tough against the solution with high frequency components, e.g., waves developing steep fronts as time evolves.

7. Concluding Remarks

7.1. **Our contributions.** In this paper, we discussed the spatial discretization of the evolutionary equations with a mixed derivative.
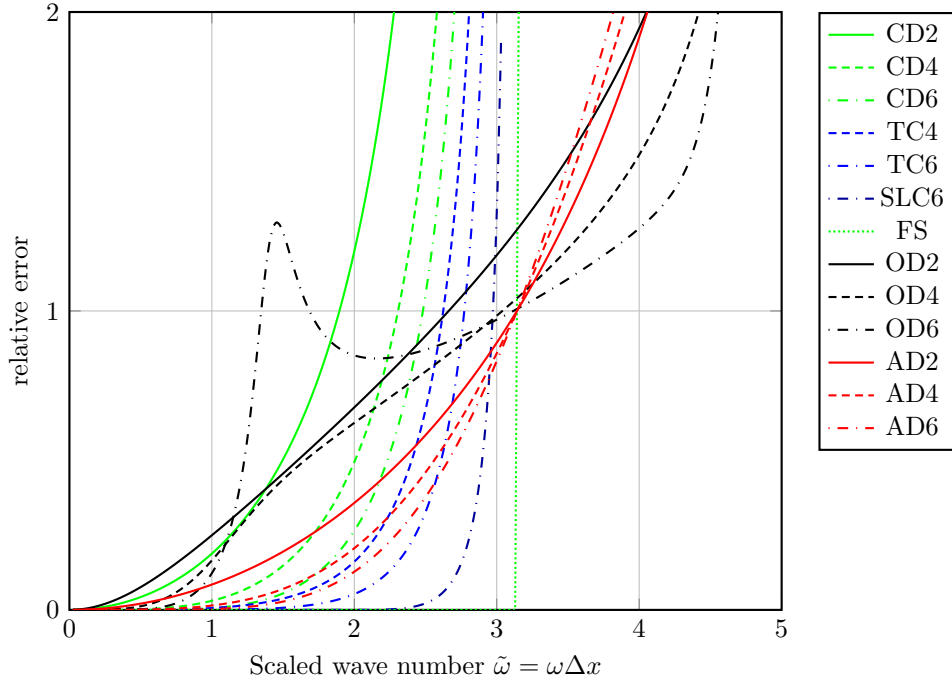
FIGURE 2. The relative errors $e(\tilde{\omega})$ of difference operators. CD, TC, SLC, FS, and OD stand for central, tridiagonal compact, spectral-like compact, Fourier-spectral, and one-sided differences. AD denotes average-difference method. The numbers attached to these names indicate the order of accuracy.

We here emphasize that, the present paper is the first attempt to construct a unified approach for (1.1) including the class (IV), while currently there are sporadic studies for each specific case in the classes (I), (II), and (III). In the proposed approach, the equivalence of the differential and integral form (Theorem 4.9) plays an important role. Though several papers dealt with each specific case in the class (II) ($\supseteq$ (I)) by following the strategy introduced by Hunter [22], in the present paper, we proposed a novel, more unified procedure, which is also applicable to the equations in the class (III) and (IV). There, we employed the Tseng generalized inverse, which is the standard concept of the generalized inverse of the linear operator between Hilbert spaces. It should be noted that, although we focused on the periodic domain in this paper, we believe that our idea to introduce the Tseng generalized inverse can be applied to other boundary conditions.

In Section 5, we investigated the difference between the discretizations of the differential and integral forms. Although most existing numerical methods have been constructed based on their integral forms for the equations in the class (II), we pointed out that the numerical solutions can violate the implicit constraint when one deal with the class (IV). In addition to that, even for the class (III) ($\supseteq$ (II) $\supseteq$ (I)), the discretization of the differential form has an advantage that is often free from nonlocal operators. Thus, we advocate employing the differential form for actual computation.

Then, in Section 6, among several finite difference methods, we concluded that the average-difference method is best suited to discretize the mixed derivative. Moreover, we developed some higher order extensions of the average-difference method, and showed this direction is promising.

7.2. **Future works.** In this paper, we left several issues to future works.

First, the rigorous justification of the infinite dimensional reduction process should be done, and we believe that it will be a powerful tool for analyzing evolutionary PDEs with a mixed derivative.

Second, although we focused only on the spatial discretization, we should also investigate how to fully discretize them. There certainly are a lot of existing works on the temporal discretization of the general implicit DAEs, but we think some special treatment will be needed when we deal with DAEs obtained by the spatial discretization of PDEs with the mixed derivative.

Third, though we used a conserved quantity in order to certify the transformation of the average-difference method for the sine-Gordon equation in Section 5.2, we did not consider any other conservation laws in this paper. In view of this, we believe that the combination of the concept of the geometric integration and the framework in this paper should be investigated.

Finally, detailed analysis and further development of the average-difference method should be discussed. For example, since the superiority of the spectral-like compact difference in low frequency components could be attributed to the fact that its parameter is defined to replicate the dispersion relation of propagating waves as good as possible, we believe that such an extension of the average-difference method may be promising. As we described in Remarks 5.1, we have already obtained some results on this issue and will report it elsewhere soon.

Acknowledgment

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