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New Conservative Schemes with Discrete Variational Derivatives for Nonlinear Wave Equations¹

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Abstract

New conservative finite difference schemes for certain classes of nonlinear wave equations are proposed. The key tool there is “discrete variational derivative,” by which discrete conservation property is realized. A similar approach for the target equations was recently proposed by Furihata, but in this paper a different approach is explored, where the target equations are first transformed to the equivalent system representations which are more natural forms to see conservation properties. Applications for the nonlinear Klein-Gordon equation and the so-called “good” Boussinesq equation are presented. Numerical examples reveal the good performance of the new schemes.

Key words: Finite-difference method, conservation, nonlinear wave equation, Boussinesq equation
1991 MSC: 65M06.

1 Introduction

The numerical integration of the 1-dimensional nonlinear wave equations of the form

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta G}{\delta u}, \quad 0 < x < L, \quad t > 0 \quad (\text{P1})$$

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and

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2}{\partial x^2} \frac{\delta G}{\delta u}, \quad 0 < x < L, \quad t > 0 \quad (\text{P2})$$

is considered, where $G(u, u_x)$ is a real-valued function of $u(x, t)$ and $u_x = \partial u / \partial x$, and

$$\frac{\delta G}{\delta u} = \frac{\partial G}{\partial u} - \frac{d}{dx} \frac{\partial G}{\partial u_x}$$

is the variational derivative of $G(u, u_x)$. The nonlinear Klein-Gordon equation, for example, belongs to (P1), and some class of the Boussinesq equations belongs to (P2). The equations of the form (P1) have in common the “energy” conservation property:

$$\frac{d}{dt} \int_0^L \left(\frac{1}{2} (u_t)^2 + G(u, u_x) \right) dx = 0, \quad (1)$$

under some suitable boundary conditions, and thus called “conservative.” The equations (P2) are also conservative, but their conservation properties are not as simple as (1). This will be discussed in the next section.

For such conservative equations, it is preferable that numerical schemes have discrete analogues of the conservation properties, since they often yield physically correct results and also numerical stability[2]. Such schemes are called “conservative schemes.” In early phase of these researches, many attempts to find conservative schemes were done independently for several specific problems; for example, conservative schemes for the nonlinear Klein-Gordon equation were studied in [1,4,11,20] (see also references in [7,17]). In the end of the twentieth century, a more unified method was given in [7,8,17], by which conservative schemes for wide range of problems can be constructed automatically. Most of specific conservative schemes in the literature then turned out to be examples of the unified approach. The method targets conservative (or dissipative, where the “energy” is monotonically dissipated along the solution) partial differential equations which is defined with variational derivative; Furihata[7] targeted real-valued equations of the form

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

which is conservative when s is odd, and dissipative otherwise; Matsuo and Furihata[17] targeted complex-valued equations of the form

$$i \frac{\partial u}{\partial t} = - \frac{\delta G}{\delta \bar{u}}, \quad \text{and} \quad \frac{\partial u}{\partial t} = - \frac{\delta G}{\delta \bar{u}},$$

which is conservative and dissipative, respectively ($\delta G / \delta \bar{u}$ is complex variational derivative); Furihata then targeted equations (P1) in [8]. In these studies the key concept is “discrete variational derivative,” which is discrete analogue

of variational derivative. The numerical scheme is then defined with it analogously to the original equation so that the discrete conservation property should be “inherited.”

There are three aims in this paper. The first aim is to introduce a new approach for the equations (P1), which is different from Furihata[8]. The key there is the fact that the equations (P1) can be represented as systems of first-order differential equations, by appropriately introducing intermediate variables. Discretizing these systems using the idea of discrete variational derivative not only gives rise to new families of conservative scheme, but brings an additional advantage that in some new schemes the time mesh size can be adaptively changed. The second aim is to cover the equations (P2), which was not covered in Furihata[8]. In particular, conservative schemes for the Boussinesq equations are obtained for the first time in the literature as far as the author knows. The third, somewhat subsidiary aim is to clarify the relation between Furihata’s approach[8] (we call it the “previous” approach throughout this paper), and the new approach. Both approaches utilizes the idea of discrete variational derivative, but start with different representations of the target equations. Then arises a natural question: do the resulting schemes by the different approaches coincide just as the continuous equations do? The “staggered grid” technique is introduced to discuss this issue.

This paper is organized as follows; in Section 2 the target equations and their properties are reviewed; Section 3 is devoted to the summary of the discrete symbols and Furihata’s previous approach; then in Section 4 the new schemes are presented and the relation between the previous and new approaches is discussed; Section 5 is for application examples where, in particular, conservative schemes for the Boussinesq equations are given; Section 6 is for concluding remarks.

2 Target equations

In this section the target equations and their properties are summarized.

2.1 Equations of the form (P1)

The equations of the form (P1) include, for example, the nonlinear Klein-Gordon equation:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \phi'(u), \quad G(u, u_x) \equiv \frac{u_x^2}{2} + \phi(u), \quad (2)$$

where $\phi'(u) = (\partial/\partial u)\phi(u)$, the Fermi-Pasta-Ulam equation:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \left(1 + \epsilon \frac{\partial u}{\partial x} \right), \quad G(u, u_x) := \frac{u_x^2}{2} + \epsilon \frac{u_x^3}{6}, \quad (3)$$

or

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \left(1 + \epsilon \left(\frac{\partial u}{\partial x} \right)^2 \right), \quad G(u, u_x) := \frac{u_x^2}{2} + \epsilon \frac{u_x^4}{12}, \quad (4)$$

and the string vibration equation:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left(\frac{\partial u / \partial x}{\sqrt{1 + (\partial u / \partial x)^2}} \right), \quad G(u, u_x) := \sqrt{1 + u_x^2}. \quad (5)$$

The solutions to the equations (P1) satisfy the following conservation property (see, for example, Furihata[8]).

Proposition 1 *Along the solution $u(x, t)$ to the equation (P1), the conservation property (1) holds if the boundary conditions satisfy*

$$\left[\frac{\partial G}{\partial u_x} u_t \right]_0^L = 0. \quad (6)$$

The assumption (6) is satisfied, for example, by the Dirichlet conditions (then $u_t = 0$ at boundaries), or if u , u_x , and u_t are periodic.

An important fact about the equations (P1) is that they can be represented as a system of equations

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \tilde{G}}{\delta u} \\ \frac{\delta \tilde{G}}{\delta v} \end{pmatrix}, \quad \text{where} \quad \tilde{G}(u, u_x, v) := \frac{v^2}{2} + G(u, u_x), \quad (\text{P1s})$$

and $v = u_t$ is an intermediate function. We call $\tilde{G}(v, u, u_x)$ the “modified” energy function. If we employ this system representation, the conservation property (1) is rewritten as the *modified* energy conservation property:

$$\frac{d}{dt} \int_0^L \tilde{G} dx = 0, \quad (7)$$

under the same assumption (6). Note that the nonlinear wave equation (P1) is usually equipped with the initial conditions $u(x, 0) = u_0(x)$, $u_t(x, 0) = u_1(x)$. Then they can be directly used as the initial conditions for the system (P1s); $u(x, 0) = u_0(x)$, $v(x, 0) = u_1(x)$.

2.2 Equations of the form (P2)

The equations of the form (2) include the “good” Boussinesq equation:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2}{\partial x^2} (u - u_{xx} + u^2), \quad G(u, u_x) := \frac{u^2}{2} + \frac{u_x^2}{2} + \frac{u^3}{3}, \quad (8)$$

and also the “bad” Boussinesq equation:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2}{\partial x^2} (u + u_{xx} + u^2), \quad G(u, u_x) := \frac{u^2}{2} - \frac{u_x^2}{2} + \frac{u^3}{3}. \quad (9)$$

To see the conservation property of (P2), it is convenient to first move to the system representation:

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \tilde{G}}{\delta u} \\ \frac{\delta \tilde{G}}{\delta v} \end{pmatrix}, \quad (\text{P2s})$$

where the intermediate function v is defined by $v_x = u_t$. Then the corresponding conservation property is presented as follows.

Proposition 2 *Along the solution to the equation (P2), or equivalently (P2s), the conservation property:*

$$\frac{d}{dt} \int_0^L \tilde{G}(v, u, u_x) dx = \frac{d}{dt} \int_0^L \left(\frac{1}{2} v^2 + G(u, u_x) \right) dx = 0 \quad (10)$$

holds under the boundary conditions which satisfy (6) and

$$\left[v \frac{\delta G}{\delta u} \right]_0^L = 0. \quad (11)$$

The conditions (6) and (11) are satisfied, for example, when $u, u_x, u_{xx}, u_t = v_x$, and v are periodic. Suppose that originally in (P2) the initial conditions $u(x, 0) = u_0(x)$, and $u_t(x, 0) = u_1(x)$ are set. The missing initial condition for v is then obtained by $v(x, 0) = \int_0^x u_1(x) dx$. Note that, in order to see the conservation property, it is more convenient to work with the system representation (P2s) than (P2), because it is not easy to replace v in (10) with u .

Remark 3 The linear wave equation: $\partial^2 u / \partial t^2 = \partial^2 u / \partial x^2$, and the linear thin film wave equation: $\partial^2 u / \partial t^2 = -\partial^4 u / \partial x^4$, can be considered as examples of both (P1) and (P2).

3 Furihata's approach

In this section, the discrete symbols used in this paper and the previous approach by Furihata[8] are summarized.

3.1 Discrete operators and formula

Numerical solution is denoted by

$$U_k^{(m)} \simeq u(k\Delta x, m\Delta t), \quad 0 \leq k \leq N, \quad m = 0, 1, 2, \dots,$$

where N is the number of space mesh points (i.e. $\Delta x = L/N$), and Δt is the time-mesh size. It is also written as $\mathbf{U}^{(m)} = (U_0^{(m)}, \dots, U_N^{(m)})^T$. The superscript (m) may be omitted where no confusion occurs. We use the standard shift operators: $s_k^{(0)} \equiv 1$, $s_k^+ f_k \equiv f_{k+1}$, $s_k^- f_k \equiv f_{k-1}$, and $s_k^{(1)} f_k \equiv (f_{k+1} + f_{k-1})/2$; the mean operators: $\mu_k^+ f_k \equiv (f_{k+1} + f_k)/2$, $\mu_k^- f_k \equiv (f_k + f_{k-1})/2$, and $\mu_k^{(1)} f_k \equiv (f_{k+1} + f_{k-1})/2$; and the difference operators: $\delta_k^{(0)} \equiv 1$, $\delta_k^+ f_k \equiv (f_{k+1} - f_k)/\Delta x$, $\delta_k^- f_k \equiv (f_k - f_{k-1})/\Delta x$, $\delta_k^{(1)} f_k \equiv (f_{k+1} - f_{k-1})/2\Delta x$, $\delta_k^{(2)} f_k \equiv (f_{k+1} - 2f_k + f_{k-1})/\Delta x^2$. Here we emphasize an identity $\delta_k^+(\delta_k^- f_k) = \delta_k^-(\delta_k^+ f_k) = \delta_k^{(2)} f_k$, which is frequently used in what follows. In the above operators, the subscript k denotes that they operate on the spatial index k . The similar operators with subscript m are also used which operate on the temporal index m ; they are defined exactly the same as above. As a discretization of integral, the trapezoidal rule is used:

$$\sum_{k=0}^N f_k \Delta x \equiv \left(\frac{1}{2} f_0 + \sum_{k=1}^N f_k + \frac{1}{2} f_N \right) \Delta x. \quad (12)$$

As to the summation rule, the following summation-by-parts formula holds:

Proposition 4 (Summation-by-parts formula)

$$\sum_{k=0}^N f_k (\delta_k^+ g_k) \Delta x + \sum_{k=0}^N (\delta_k^- f_k) g_k \Delta x = \left[\frac{f_k (s_k^+ g_k) + (s_k^- f_k) g_k}{2} \right]_0^N. \quad (\text{SBP})$$

3.2 Two-point discrete variational derivative

In this and the subsequent subsection, “discrete variational derivatives” are defined. Suppose the energy function $G(u, u_x)$ be of the form

$$G(u, u_x) = \sum_{l=1}^M f_l(u) g_l(u_x), \quad M \in \{1, 2, \dots\}. \quad (13)$$

Observe that all G in the previous section fall into this category; for example, for the nonlinear Klein-Gordon equation, $M = 2$, $f_1(u) = 1$, $g_1(u_x) =$

$u_x^2/2$, $f_2(u) = \phi(u)$, and $g_2(u_x) = 1$. Analogously, suppose the discrete analogue of the energy be given in the form

$$G_{d,k}(\mathbf{U}^{(m)}) = \sum_{l=1}^M f_l(U_k^{(m)}) g_l^+(\delta_k^+ U_k^{(m)}) g_l^-(\delta_k^- U_k^{(m)}), \quad 0 \leq k \leq N. \quad (14)$$

(see also Section 5 for the concrete examples of G_d). The discrete energy $G_{d,k}$ is a real-valued scalar function of $\mathbf{U}^{(m)}$ which approximates $G(u, u_x)$ at $x = k\Delta x$, $t = m\Delta t$. We also write $G_d(\mathbf{U}^{(m)})$ as a vector function.

Now recall the continuous variation calculation:

$$\begin{aligned} & \int_0^L (G(u + \delta u, u_x + \delta u_x) - G(u, u_x)) dx \\ &= \int_0^L \left(\frac{\partial G}{\partial u} \delta u + \frac{\partial G}{\partial u_x} \delta u_x \right) dx + O(\delta u^2) \\ &= \int_0^L \frac{\delta G}{\delta u} dx + \left[\frac{\partial G}{\partial u_x} \delta u \right]_0^L + O(\delta u^2). \end{aligned} \quad (15)$$

With a given discrete energy function (14), a discrete analogue of (15) becomes as follows.

$$\begin{aligned} & \sum_{k=0}^N \left(G_{d,k}(\mathbf{U}^{(m+1)}) - G_{d,k}(\mathbf{U}^{(m)}) \right) \Delta x = \\ & \sum_{k=0}^N \left[\left(\frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) (U_k^{(m+1)} - U_k^{(m)}) \right] \Delta x + B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}), \end{aligned} \quad (16)$$

where $\delta G_d / \delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})$ is an approximation of $\delta G / \delta u$, and hence called the “discrete variational derivative” of G_d . More exactly, it is called “two-points” discrete variational derivative, since it refers two approximate solutions $\mathbf{U}^{(m+1)}$ and $\mathbf{U}^{(m)}$, when we are in need of distinguishing it from the “three-points” discrete variational derivative introduced in the next subsection. The discrete quantities appearing in (16) is defined as

$$\begin{aligned} \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} &: \equiv \frac{\partial G_d}{\partial(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} - \delta_k^- \left(\frac{\partial G_d}{\partial \delta^+(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \\ &\quad - \delta_k^+ \left(\frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right), \end{aligned} \quad (17)$$

$$\begin{aligned}
B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) &:= \frac{1}{2} \left[\frac{\partial G_d}{\partial \delta^+(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} (s_k^+(U_k^{(m+1)} - U_k^{(m)})) \right. \\
&\quad + \left\{ s_k^- \left(\frac{\partial G_d}{\partial \delta^+(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \right\} (U_k^{(m+1)} - U_k^{(m)}) \\
&\quad + \frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} (s_k^-(U_k^{(m+1)} - U_k^{(m)})) \\
&\quad \left. + \left\{ s_k^+ \left(\frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \right\} (U_k^{(m+1)} - U_k^{(m)}) \right]_0^N, \quad (18)
\end{aligned}$$

where

$$\begin{aligned}
\frac{\partial G_d}{\partial (\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} &:= \sum_{l=1}^M \left(\frac{f_l(U_k^{(m+1)}) - f_l(U_k^{(m)})}{U_k^{(m+1)} - U_k^{(m)}} \right) \\
&\quad \times \left(\frac{g_l^+(\delta_k^+ U_k^{(m+1)}) g_l^-(\delta_k^- U_k^{(m+1)}) + g_l^+(\delta_k^+ U_k^{(m)}) g_l^-(\delta_k^- U_k^{(m)})}{2} \right), \quad (19a)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} &:= \sum_{l=1}^M \left(\frac{f_l(U_k^{(m+1)}) + f_l(U_k^{(m)})}{2} \right) \\
&\quad \times \left(\frac{g_l^+(\delta_k^+ U_k^{(m+1)}) + g_l^+(\delta_k^+ U_k^{(m)})}{2} \right) \left(\frac{g_l^-(\delta_k^- U_k^{(m+1)}) - g_l^-(\delta_k^- U_k^{(m)})}{\delta_k^-(U_k^{(m+1)} - U_k^{(m)})} \right) \quad (19b)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial G_d}{\partial \delta^+(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} &:= \sum_{l=1}^M \left(\frac{f_l(U_k^{(m+1)}) + f_l(U_k^{(m)})}{2} \right) \\
&\quad \times \left(\frac{g_l^-(\delta_k^- U_k^{(m+1)}) + g_l^-(\delta_k^- U_k^{(m)})}{2} \right) \left(\frac{g_l^+(\delta_k^+ U_k^{(m+1)}) - g_l^+(\delta_k^+ U_k^{(m)})}{\delta_k^+(U_k^{(m+1)} - U_k^{(m)})} \right) \quad (19c)
\end{aligned}$$

which are discrete approximations to $\partial G/\partial u$, $\partial G/\partial u_x$, respectively. The identity (16) can be verified by some calculations with (SBP).

Remark 5 In the definitions definition (19a), the quantity $(f_l(U_k^{(m+1)}) - f_l(U_k^{(m)}))/(U_k^{(m+1)} - U_k^{(m)})$ with $U_k^{(m+1)} = U_k^{(m)}$ is defined by $f_l'(U_k^{(m)})$, where $(\cdot)'$ denotes differentiation. This notice applies to all the similar expressions.

3.3 Three-points discrete variational derivative

Suppose the energy G be given in the form (13). Analogously, suppose a discrete energy be given in the form

$$G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) = \sum_{l=1}^M f_l(U_k^{(m+1)}, U_k^{(m)}) g_l^+(\delta_k^+ U_k^{(m+1)}, \delta_k^+ U_k^{(m)}) g_l^-(\delta_k^- U_k^{(m+1)}, \delta_k^- U_k^{(m)}). \quad (20)$$

Observe that, in contrast to (14), this discrete energy refers *two* approximate solutions. Like as in the previous subsection, with the discrete energy a discrete analogue of (15) can be given as follows.

$$\begin{aligned} & \sum_{k=0}^N \left(G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) - G_{d,k}(\mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}) \right) \Delta x \\ &= \sum_{k=0}^N \left[\frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \left(\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2} \right) \right] \Delta x \\ & \quad + B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}). \end{aligned} \quad (21)$$

We call the discrete quantity $\delta G_d / \delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k$ the “three-points discrete variational derivative,” since it refers three approximate solutions. The discrete quantities in above identity are defined as follows.

$$\begin{aligned} & \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} := \frac{\partial G_d}{\partial(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \\ & \quad - \delta_k^- \left(\frac{\partial G_d}{\partial \delta^+(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \right) \\ & \quad - \delta_k^+ \left(\frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \right), \end{aligned} \quad (22)$$

$$\begin{aligned} & B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}) := \\ & \frac{\Delta t}{2} \left[\frac{\partial G_d}{\partial(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \left\{ s_k^+ \left(\delta_m^{(1)} U_k^{(m)} \right) \right\} \right. \\ & \quad + \left\{ s_k^- \left(\frac{\partial G_d}{\partial(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \right) \right\} \left(\delta_m^{(1)} U_k^{(m)} \right) \\ & \quad + \frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \left\{ s_k^- \left(\delta_m^{(1)} U_k^{(m)} \right) \right\} \\ & \quad \left. + \left\{ s_k^+ \left(\frac{\partial G_d}{\partial \delta^-(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \right) \right\} \left(\delta_m^{(1)} U_k^{(m)} \right) \right]_0^N, \end{aligned} \quad (23)$$

$$\begin{aligned} & \frac{\partial G_d}{\partial(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} = \sum_{l=1}^M \frac{f_l^{(m,m+1)} - f_l^{(m,m-1)}}{\frac{1}{2}(U_k^{(m+1)} - U_k^{(m-1)})} \\ & \quad \times \left(\frac{g_l^{+, (m,m+1)} g_l^{-, (m,m+1)} + g_l^{+, (m,m-1)} g_l^{-, (m,m-1)}}{2} \right), \end{aligned} \quad (24a)$$

$$\begin{aligned}
\frac{\partial G_d}{\partial \delta^\pm(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} = & \\
& \sum_{l=1}^M \left(\frac{f_l^{(m,m+1)} + f_l^{(m,m-1)}}{2} \right) \left(\frac{g_l^{\mp,(m,m+1)} + g_l^{\mp,(m,m-1)}}{2} \right) \\
& \times \left(\frac{g_l^{\pm,(m,m+1)} - g_l^{\pm,(m,m-1)}}{\frac{1}{2}\delta_k^\pm(U_k^{(m+1)} - U_k^{(m-1)})} \right). \tag{24b}
\end{aligned}$$

In above definition the abbreviations $f_l^{(m,m+1)} \equiv f_l(U_k^{(m+1)}, U_k^{(m)})$, $g_l^{\pm,(m,m+1)} \equiv g_l^\pm(\delta_k^\pm U_k^{(m+1)}, \delta_k^\pm U_k^{(m)})$, and so on, are used to simplify the notation. The double signs correspond. The identity (21) can be verified by some calculations with (SBP).

Remark 6 The three-points discrete variational derivative defined here is a special case of Furihata's "four-points" discrete variational derivative[8], where two of the referred four approximate solutions are identical.

3.4 Conservative schemes by the previous approach

With the two-points or three-points discrete variational derivatives defined above, Furihata[8] proposed the following schemes for the equation (P1).

Scheme 1 (Implicit scheme for (P1)) For a given set of initial data $\mathbf{U}^{(0)}, \mathbf{U}^{(1)}$, we compute $\mathbf{U}^{(m)} (m = 2, 3, \dots)$ by

$$\delta_m^{(2)} U_k^{(m)} = - \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k}, \quad 0 \leq k \leq N. \tag{25}$$

The initial data $\mathbf{U}^{(0)}$ is obtained from the initial data $u(x, 0)$, and $\mathbf{U}^{(1)}$ from $u(x, 0)$ and $u_t(x, 0)$, using some other numerical schemes. This notice also applies to all the schemes in this paper. The discrete variational derivative in the right hand side generally includes the second-order difference operator $\delta_k^{(2)}$, which corresponds to $\partial^2/\partial x^2$, and thus possibly refers *outside* the defined region $0 \leq k \leq N$ (see the examples in Section 5). The undefined values are assumed to be resolved by some discrete boundary conditions. The discrete boundary conditions are also assumed to satisfy a certain condition so that the scheme becomes conservative.

Proposition 7 (Conservation property of Scheme 1) Suppose that discrete boundary conditions are imposed so that $B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}) = 0$ ($m = 1, 2, 3, \dots$). Then Scheme 1 is conservative in the sense

$$\begin{aligned}
& \sum_{k=0}^N \left\{ \frac{(\delta_m^+ U_k^{(m)})^2}{2} + G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) \right\} \Delta x \\
&= \sum_{k=0}^N \left\{ \frac{(\delta_m^+ U_k^{(0)})^2}{2} + G_{d,k}(\mathbf{U}^{(1)}, \mathbf{U}^{(0)}) \right\} \Delta x,
\end{aligned} \tag{26}$$

for $m = 1, 2, \dots$, holds.

Scheme 2 (Explicit scheme for (P1)) For a given set of initial data $\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{U}^{(2)}$, we compute $\mathbf{U}^{(m)}$ ($m = 1, 2, \dots$) by

$$\frac{U_k^{(m+2)} - U_k^{(m+1)} - U_k^{(m)} + U_k^{(m-1)}}{2\Delta t} = -\frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k}, \quad 0 \leq k \leq N. \tag{27}$$

Proposition 8 (Conservation property of Scheme 2) Suppose that discrete boundary conditions are imposed so that $B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) = 0$ ($m = 1, 2, 3, \dots$). Then Scheme 2 is conservative in the sense

$$\begin{aligned}
& \sum_{k=0}^N \left\{ \frac{(\delta_m^+ U_k^{(m)})(\delta_m^- U_k^{(m)})}{2} + G_{d,k}(\mathbf{U}^{(m)}) \right\} \Delta x \\
&= \sum_{k=0}^N \left\{ \frac{(\delta_m^+ U_k^{(1)})(\delta_m^- U_k^{(1)})}{2} + G_{d,k}(\mathbf{U}^{(1)}) \right\} \Delta x,
\end{aligned} \tag{28}$$

holds for $m = 2, 3, \dots$

4 New approach based on the system representations

New schemes based on the representations (P1s) and (P2s) are proposed. To this end, the idea of discrete variational derivative is first extended to multivariate function \tilde{G} (see Matsuo[14] for complete treatment of general multivariate energy function). Furthermore, the relation between the previous and new approaches is discussed.

4.1 Discrete variational derivatives for multivariate energy function \tilde{G}

In this subsection, four different discrete variational derivatives for four different discretizations of the energy \tilde{G} are presented. Note that the following variation calculation holds in continuous context.

$$\begin{aligned}
& \int_0^L \left(\tilde{G}(v + \delta v, u + \delta u, u_x + \delta u_x) - \tilde{G}(v, u, u_x) \right) dx \\
&= \int_0^L \left(\frac{\delta \tilde{G}}{\delta v} + \frac{\delta \tilde{G}}{\delta u} \right) dx + \left[\frac{\partial \tilde{G}}{\partial u_x} \delta u \right]_0^L + O(\delta u^2) + O(\delta v^2).
\end{aligned} \tag{29}$$

Recall the definition $\tilde{G}(v, u, u_x) = v^2/2 + G(u, u_x)$. Since this \tilde{G} does not depend on v_x , there is no boundary term as to v in (29). Though the derivative $\delta \tilde{G}/\delta v$ is just v in this case, we prefer to leave it since it clarifies the variational structure. Since \tilde{G} is separable into u parts v parts, $\delta \tilde{G}/\delta u$ and $\partial \tilde{G}/\partial u_x$ are identical to $\delta G/\delta u$ and $\partial G/\partial u_x$, respectively.

4.1.1 Two-points discrete variational derivative for \tilde{G}

Suppose the discrete modified energy function be of the form

$$\tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)}) = \frac{(V_k^{(m)})^2}{2} + G_{d,k}(\mathbf{U}^{(m)}). \tag{30}$$

The following is a multivariate extension of the discrete variation identity (16).

Lemma 9 (Discrete variation identity I for \tilde{G}) *As to the discrete modified energy function \tilde{G}_d defined in (30), the discrete variation identity holds:*

$$\begin{aligned}
& \sum_{k=0}^N \left(\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{V}^{(m+1)}) - \tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)}) \right) \Delta x = \\
& \sum_{k=0}^N \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) (U_k^{(m+1)} - U_k^{(m)}) \right. \\
& \quad \left. + \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) (V_k^{(m+1)} - V_k^{(m)}) \right] \Delta x + B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}), \tag{31}
\end{aligned}$$

where

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} = \frac{V_k^{(m+1)} + V_k^{(m)}}{2}, \tag{32}$$

and

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} = \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \tag{33}$$

is what defined in (16).

PROOF. The modified energy function $\tilde{G}_{d,k}$ is separable into $U_k^{(m)}$ parts and $V_k^{(m)}$ part, and they can be considered independently. For $U_k^{(m)}$ parts, i.e. $G_d(\mathbf{U}^{(m)})$, the discrete variation identity (16) holds. For $V_k^{(m)}$ part,

$$\begin{aligned}
& \sum_{k=0}^N \left(\frac{(V_k^{(m+1)})^2}{2} - \frac{(V_k^{(m)})^2}{2} \right) \Delta x \\
&= \sum_{k=0}^N \left(\frac{V_k^{(m+1)} + V_k^{(m)}}{2} \right) (V_k^{(m+1)} - V_k^{(m)}) \Delta x \\
&= \sum_{k=0}^N \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} (V_k^{(m+1)} - V_k^{(m)}) \Delta x.
\end{aligned} \tag{34}$$

□

4.1.2 Three-points discrete variational derivative for \tilde{G}

Suppose the discrete modified energy function be of the form

$$\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}) = \frac{V_k^{(m+1)} V_k^{(m)}}{2} + G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}). \tag{35}$$

The following is a multivariate extension of the discrete variation identity (21).

Lemma 10 (Discrete variation identity II for \tilde{G}) *As to the discrete modified energy function \tilde{G}_d defined in (35), the discrete variation identity holds:*

$$\begin{aligned}
& \sum_{k=0}^N \left(G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}) - G_{d,k}(\mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}, \mathbf{V}^{(m)}, \mathbf{V}^{(m-1)}) \right) \Delta x \\
&= \sum_{k=0}^N \left[\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \left(\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2} \right) \right. \\
&\quad \left. \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}, \mathbf{V}^{(m-1)})_k} \left(\frac{V_k^{(m+1)} - V_k^{(m-1)}}{2} \right) \right] \Delta x \\
&\quad + B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}), \tag{36}
\end{aligned}$$

where

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}, \mathbf{V}^{(m-1)})_k} = V_k^{(m)}, \tag{37}$$

and

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} = \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \tag{38}$$

is what defined in (21).

PROOF. For the $U_k^{(m)}$ part, the discrete variation identity (21) holds. For the $V_k^{(m)}$ part,

$$\begin{aligned}
& \sum_{k=0}^N \left(\frac{V_k^{(m+1)} V_k^{(m)}}{2} - \frac{V_k^{(m)} V_k^{(m-1)}}{2} \right) \Delta x \\
&= \sum_{k=0}^N V_k^{(m)} \left(\frac{V_k^{(m+1)} - V_k^{(m-1)}}{2} \right) \Delta x \\
&= \sum_{k=0}^N \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}, \mathbf{V}^{(m-1)})_k} \left(\frac{V_k^{(m+1)} - V_k^{(m-1)}}{2} \right) \Delta x.
\end{aligned} \tag{39}$$

□

Remark 11 If \tilde{G}_d is defined by

$$\begin{aligned}
\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}) &= \frac{(V_k^{(m+1)})^2 + (V_k^{(m)})^2}{2} \\
&+ G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}),
\end{aligned} \tag{40}$$

then

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}, \mathbf{V}^{(m-1)})_k} = \frac{V_k^{(m+1)} + V_k^{(m-1)}}{2}, \tag{41}$$

and a slightly different discrete variation identity are obtained.

4.1.3 Discrete variational derivative for \tilde{G} using staggered mesh points

So far only the integral time mesh $m\Delta t$ ($m = 0, 1, 2, \dots$) has been considered. Now let us also consider the “staggered” time mesh $(m + 1/2)\Delta t$ ($m = 0, 1, 2, \dots$), and approximate the intermediate function v on this staggered time mesh. This approximate solution is denoted by $\mathbf{V}^{(m+\frac{1}{2})}$. Two new discrete variational derivatives for \tilde{G} are presented below.

Firstly, suppose the discrete modified energy function be of the form

$$\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})}) = \frac{\left(V_k^{(m+\frac{1}{2})}\right)^2}{2} + G_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}). \tag{42}$$

Observe this refers two approximate solutions $U_k^{(m+1)}, U_k^{(m)}$ in u parts, while only one solution $V_k^{(m+\frac{1}{2})}$ in v part. This is in contrast to the definition (30) (or (35), respectively), which in both u and v parts refers one (or two) approximate solution(s). The next lemma holds as to the discrete energy (42).

Lemma 12 (Discrete variation identity III for \tilde{G}) *As to the discrete modified energy function \tilde{G}_d defined in (42), the discrete variation identity holds:*

$$\begin{aligned}
& \sum_{k=0}^N \left(\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})}) - \tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}, \mathbf{V}^{(m-\frac{1}{2})}) \right) \Delta x \\
&= \sum_{k=0}^N \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \right) (U_k^{(m+1)} - U_k^{(m-1)}) \right. \\
&\quad \left. + \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} \right) (V_k^{(m+\frac{1}{2})} - V_k^{(m-\frac{1}{2})}) \right] \Delta x \\
&\quad + B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}), \tag{43}
\end{aligned}$$

where

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} = \frac{V_k^{(m+\frac{1}{2})} + V_k^{(m-\frac{1}{2})}}{2}, \tag{44}$$

and

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} = \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} \tag{45}$$

is what defined in (21).

PROOF. For the u part, the proof is similar to Lemma 10. The v part is similar to Lemma 9. \square

Secondly, suppose the discrete modified energy function be of the form

$$\tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})}) = \frac{V_k^{(m+\frac{1}{2})} V_k^{(m-\frac{1}{2})}}{2} + G_{d,k}(\mathbf{U}^{(m)}). \tag{46}$$

This is in contrast with (42); now it refers *one* approximate solution for u and *two* solutions for v . For the discrete energy, the following lemma holds.

Lemma 13 (Discrete variation identity IV for \tilde{G}) *As to the discrete modified energy function \tilde{G}_d defined in (46), the discrete variation identity holds:*

$$\begin{aligned}
& \sum_{k=0}^N \left(\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}) - \tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})}) \right) \Delta x \\
&= \sum_{k=0}^N \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) (U_k^{(m+1)} - U_k^{(m)}) \right. \\
&\quad \left. + \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} \right) (V_k^{(m+\frac{3}{2})} - V_k^{(m-\frac{1}{2})}) \right] \Delta x \\
&\quad + B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}), \tag{47}
\end{aligned}$$

where

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} = V_k^{(m+\frac{1}{2})}, \quad (48)$$

and

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} = \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \quad (49)$$

is what defined in (16).

PROOF. For the u part, the proof is similar to Lemma 9. The v part is similar to Lemma 10. \square

4.2 New schemes for the equation (P1s)

With the discrete variational derivatives for the modified energy function \tilde{G} , four new schemes for (P1s) are presented, each of which is derived from the corresponding one of the discrete variations Lemma 9, 10, 12, and 13.

Scheme 3 (New implicit scheme I for (P1s)) *Let $\tilde{G}_{d,k}$ be what defined in (30), and corresponding discrete variational derivative in Lemma 9. Then for a given set of initial data $\mathbf{U}^{(0)}, \mathbf{V}^{(0)}$, we compute $\mathbf{U}^{(m)}, \mathbf{V}^{(m)}$ ($m = 1, 2, \dots$) by*

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} = \frac{V_k^{(m+1)} + V_k^{(m)}}{2}, \quad (50a)$$

$$\frac{V_k^{(m+1)} - V_k^{(m)}}{\Delta t} = -\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k}, \quad (50b)$$

for $0 \leq k \leq N$.

Theorem 14 (Conservation property of Scheme 3) *Suppose that discrete boundary conditions which satisfy $B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) = 0$ ($m = 0, 1, \dots$) are imposed. Then Scheme 3 is conservative in the sense*

$$\sum_{k=0}^N {}''\tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)})\Delta x = \sum_{k=0}^N {}''\tilde{G}_{d,k}(\mathbf{U}^{(0)}, \mathbf{V}^{(0)})\Delta x \quad m = 1, 2, \dots, \quad (51)$$

holds.

PROOF. By the assumption on the boundary conditions, and from Lemma 9,

$$\begin{aligned}
& \frac{1}{\Delta t} \sum_{k=0}^N \left(\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{V}^{(m+1)}) - \tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)}) \right) \Delta x \\
&= \sum_{k=0}^N \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} \right) \right. \\
&\quad \left. + \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \left(\frac{V_k^{(m+1)} - V_k^{(m)}}{\Delta t} \right) \right] \Delta x \\
&= \sum_{k=0}^N \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \right. \\
&\quad \left. - \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \right] \Delta x \\
&= 0.
\end{aligned} \tag{52}$$

□

Scheme 4 (New explicit scheme I for (P1s)) Let $\tilde{G}_{d,k}$ be what defined in (35), and corresponding discrete variational derivative in Lemma 10. Then for a given set of initial data $\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{V}^{(0)}, \mathbf{V}^{(1)}$, we compute $\mathbf{U}^{(m)}, \mathbf{V}^{(m)}$ ($m = 2, 3, \dots$) by

$$\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2\Delta t} = \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}, \mathbf{V}^{(m-1)})_k} = V_k^{(m)}, \tag{53a}$$

$$\frac{V_k^{(m+1)} - V_k^{(m-1)}}{2\Delta t} = -\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k}, \tag{53b}$$

for $0 \leq k \leq N$.

Theorem 15 (Conservation property of Scheme 4) Suppose that discrete boundary conditions which satisfy $B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}) = 0$ ($m = 1, 2, \dots$) are imposed. Then Scheme 4 is conservative in the sense

$$\sum_{k=0}^N \tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}) \Delta x = \sum_{k=0}^N \tilde{G}_{d,k}(\mathbf{U}^{(1)}, \mathbf{U}^{(0)}, \mathbf{V}^{(1)}, \mathbf{V}^{(0)}) \Delta x, \tag{54}$$

holds for $m = 1, 2, \dots$

PROOF. The proof is similar to Theorem 14, except that Lemma 10 should be used. □

Scheme 5 (New implicit scheme II for (P1s)) Let $\tilde{G}_{d,k}$ be what defined in (42), and corresponding discrete variational derivative in Lemma 12. Then

for a given set of initial data $\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{V}^{(\frac{1}{2})}$, we compute $\mathbf{U}^{(m+1)}, \mathbf{V}^{(m+\frac{1}{2})}$ ($m = 1, 2, \dots$) by

$$\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2\Delta t} = \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} = \frac{V_k^{(m+\frac{1}{2})} + V_k^{(m-\frac{1}{2})}}{2}, \quad (55a)$$

$$\frac{V_k^{(m+\frac{1}{2})} - V_k^{(m-\frac{1}{2})}}{\Delta t} = -\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k}, \quad (55b)$$

for $0 \leq k \leq N$.

Note that this scheme is implicit; first, the equations (55a) and (55b) are solved simultaneously to obtain $\mathbf{U}^{(2)}$ and $\mathbf{V}^{(\frac{3}{2})}$. Then $\mathbf{U}^{(3)}$ and $\mathbf{V}^{(\frac{5}{2})}$, and so on. Scheme 5 have the following conservation property.

Theorem 16 (Conservation property of Scheme 5) *Suppose that discrete boundary conditions which satisfy $B_2(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)}) = 0$ ($m = 1, 2, 3, \dots$) are imposed. Then Scheme 5 is conservative in the sense*

$$\sum_{k=0}^N {}''\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})})\Delta x = \sum_{k=0}^N {}''\tilde{G}_{d,k}(\mathbf{U}^{(1)}, \mathbf{U}^{(0)}, \mathbf{V}^{(\frac{1}{2})})\Delta x, \quad (56)$$

for $m = 1, 2, \dots$, holds.

PROOF. Straightforward from Lemma 12. \square

Scheme 6 (New explicit scheme II for (P1s)) *Let $\tilde{G}_{d,k}$ be what defined in (46), and corresponding discrete variational derivative in Lemma 13. Then for a given set of initial data $\mathbf{U}^{(0)}, \mathbf{V}^{(-\frac{1}{2})}, \mathbf{V}^{(\frac{1}{2})}$, we compute $\mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})}$ ($m = 1, 2, \dots$) by*

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} = V_k^{(m+\frac{1}{2})}, \quad (57a)$$

$$\frac{V_k^{(m+\frac{3}{2})} - V_k^{(m-\frac{1}{2})}}{2\Delta t} = -\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k}, \quad (57b)$$

for $0 \leq k \leq N$.

This scheme is explicit if we compute $\mathbf{U}^{(1)}, \mathbf{V}^{(\frac{3}{2})}, \mathbf{U}^{(2)}, \mathbf{V}^{(\frac{5}{2})}, \dots$ in this order. We can also start with the initial conditions $\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \mathbf{V}^{(-\frac{1}{2})}$; in this case, we compute $\mathbf{V}^{(\frac{1}{2})}, \mathbf{V}^{(\frac{3}{2})}, \mathbf{U}^{(2)}, \mathbf{V}^{(\frac{5}{2})}, \dots$, in this order. Or we can start with

$U^{(0)}, U^{(1)}, U^{(2)}$, from which we compute $V^{(\frac{1}{2})}, V^{(\frac{3}{2})}, V^{(\frac{5}{2})}, U^{(3)}, \dots$, and so on. The next conservation property holds for the scheme.

Theorem 17 (Conservation property of Scheme 6) *Suppose that discrete boundary conditions which satisfy $B_1(U^{(m+1)}, U^{(m)}) = 0$ ($m = 0, 1, 2, \dots$) are imposed. Then Scheme 6 is conservative in the sense*

$$\sum_{k=0}^N {}''\tilde{G}_{d,k}(U^{(m+1)}, V^{(m+\frac{1}{2})}, V^{(m-\frac{1}{2})})\Delta x = \sum_{k=0}^N {}''\tilde{G}_{d,k}(U^{(0)}, V^{(\frac{1}{2})}, V^{(-\frac{1}{2})})\Delta x, \quad (58)$$

for $m = 1, 2, \dots$, holds.

PROOF. Straightforward from Lemma 13. \square

Remark 18 Another new scheme is derived from the fifth discrete variation identity pointed out in Remark 11. The scheme, however, seems to have no special advantage over other schemes, and thus is not discussed any further in this paper.

4.3 Relation between the previous and new approaches

Now we have two *previous* schemes: Scheme 1 and Scheme 2, and four *new* schemes: Scheme 3, 4, 5, and 6, for the equations (P1), or equivalently (P1s). In this subsection, the relations between these schemes are discussed.

Scheme 1 can be regarded as the special case of Scheme 5 as follows.

Theorem 19 (Coincidence of Scheme 1 and 5) *Scheme 5 reduces to Scheme 1 if the initial conditions imposed on Scheme 5 satisfy*

$$\frac{U_k^{(1)} - U_k^{(0)}}{\Delta t} = V_k^{(\frac{1}{2})}. \quad (59)$$

PROOF. Observe that the equation (55a) is equivalent to

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{2\Delta t} + \frac{U_k^{(m)} - U_k^{(m-1)}}{2\Delta t} = \frac{V_k^{(m+\frac{1}{2})}}{2} + \frac{V_k^{(m-\frac{1}{2})}}{2}. \quad (60)$$

Then by induction

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = V_k^{(m+\frac{1}{2})} \quad (55a')$$

holds for $m = 1, 2, \dots$, under the assumption (59). Subtracting (55a') with m from $m + 1$ and dividing by Δt , we obtain

$$\delta_m^{(2)} U_k^{(m)} = \frac{V_k^{(m+\frac{1}{2})} - V_k^{(m-\frac{1}{2})}}{\Delta t} = -\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k}. \quad (61)$$

This coincides with Scheme 1, since as pointed above

$$\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k} = \frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k}. \quad (62)$$

□

Scheme 5 needs *three* initial conditions: $\mathbf{U}^{(0)}$, $\mathbf{U}^{(1)}$, and $\mathbf{V}^{(\frac{1}{2})}$, while Scheme 1 needs only *two*: $\mathbf{U}^{(0)}$ and $\mathbf{U}^{(1)}$. It is quite natural to generate the missing third condition for $\mathbf{V}^{(\frac{1}{2})}$ by (59); then Scheme 5 reduces to Scheme 1. On the other hand, it is still possible to somehow find $\mathbf{V}^{(\frac{1}{2})}$, for example by another numerical algorithm, which does not satisfy the assumption (59); then Scheme 5 generates approximate solutions which Scheme 1 never generates.

As to Scheme 2 and 6, the next result holds.

Theorem 20 (Coincidence of Scheme 2 and 6) *If we start with the initial conditions $\mathbf{U}^{(0)}$, $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$, then Scheme 6 coincides with Scheme 2.*

PROOF. Subtracting the equations (57a) with $m - 1$ from $m + 1$ and dividing by $2\Delta t$, we obtain

$$\frac{U_k^{(m+2)} - U_k^{(m+1)} - U_k^{(m)} + U_k^{(m-1)}}{2\Delta t} = \frac{V_k^{(m+\frac{3}{2})} - V_k^{(m-\frac{1}{2})}}{2\Delta t} = -\frac{\delta G_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k}, \quad (63)$$

which coincides Scheme 2. □

Both Scheme 2 and 6 need three initial conditions to start. Thus there is no ambiguous free parameter as in the previous theorem which makes the difference.

As a result, a conclusion is obtained that the new approach based on the system representation (P1s) includes, and thus more general than, the previous approach. This encourages us to work with the system representation, because it provides wider variety of schemes. The new schemes, however, are not necessarily *superior*; actually, Scheme 4 seems to be less practical than Scheme 2

if we rewrite it as

$$\frac{U_k^{(m+2)} - 2U_k^{(m)} + U_k^{(m-2)}}{(2\Delta t)^2} = -\frac{\delta\tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{U}^{(m-1)})_k}, \quad (64)$$

which is obtained from (57b), and unnecessarily broader than Scheme 2.

Notice also that Scheme 3 is a one-step method, and thus can be implemented using some adaptive time mesh control strategy. Even in such circumstances the conservation property (Theorem 14) is not destroyed. This is another remarkable advantage of the new approach. Scheme 5 can be also adaptively implemented if the initial conditions satisfy (59) and thus the scheme is reduced to one-step form with (55a').

4.4 New schemes for the equation (P2s)

By slightly modifying Scheme 3, 4, 5, and 6, four new schemes for the equation (P2s) can be derived. Two of them are explicitly presented here. The other two can be derived similarly.

The following scheme is based on Scheme 3.

Scheme 7 (New implicit scheme for (P2s)) *Let $\tilde{G}_{d,k}$ be what defined in (30), and corresponding discrete variational derivative in Lemma 9. Then for a given set of initial data $\mathbf{U}^{(0)}, \mathbf{V}^{(0)}$, we compute $\mathbf{U}^{(m)}, \mathbf{V}^{(m)}$ ($m = 1, 2, \dots$) by*

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = \delta_k^+ \left(\frac{\delta\tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) = \delta_k^+ \left(\frac{V_k^{(m+1)} + V_k^{(m)}}{2} \right), \quad (65a)$$

$$\frac{V_k^{(m+1)} - V_k^{(m)}}{\Delta t} = \delta_k^- \left(\frac{\delta\tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right), \quad (65b)$$

for $0 \leq k \leq N$.

Theorem 21 (Conservation property of Scheme 7) *Suppose that imposed discrete boundary conditions satisfy $B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) = 0$ and*

$$\left[\frac{\delta\tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \cdot s_k^+ \left(\frac{\delta\tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) + \left(s_k^- \frac{\delta\tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \frac{\delta\tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right]_0^N = 0, \quad (66)$$

for $m = 0, 1, 2, \dots$. Then Scheme 7 is conservative in the sense

$$\sum_{k=0}^N {}'' \tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)}) \Delta x = \sum_{k=0}^N {}'' \tilde{G}_{d,k}(\mathbf{U}^{(0)}, \mathbf{V}^{(0)}) \Delta x \quad m = 1, 2, \dots, \quad (67)$$

holds.

PROOF. By the assumption (66), and from Lemma 9,

$$\begin{aligned} & \frac{1}{\Delta t} \sum_{k=0}^N {}'' \left(\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{V}^{(m+1)}) - \tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)}) \right) \Delta x \\ &= \sum_{k=0}^N {}'' \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} \right) \right. \\ & \quad \left. + \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \left(\frac{V_k^{(m+1)} - V_k^{(m)}}{\Delta t} \right) \right] \Delta x \\ &= \sum_{k=0}^N {}'' \left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \delta_k^+ \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \right. \\ & \quad \left. + \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \delta_k^- \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \right] \Delta x \\ &= \frac{1}{2} \left[\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \cdot s_k^+ \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right) \right. \\ & \quad \left. + \left(s_k^- \frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} \right]_0^N \\ &= 0. \end{aligned} \quad (68)$$

In the last equality, the summation-by-parts formula (SBP) is used. \square

The assumption (66) is satisfied, for example, if both $U_k^{(m)}$ and $V_k^{(m)}$ are periodic in spatial index k . Scheme 7 may not seem symmetric because one-sided difference operators δ_k^+ , δ_k^- are used. But the reduced scheme

$$\delta_m^{(2)} U_k^{(m)} = \delta_k^{(2)} \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right), \quad (69)$$

which is obtained by subtracting the equations (65a) with m from $m+1$, is symmetric. It is also possible to replace δ_k^+ , δ_k^- with symmetric difference operator $\delta_k^{(1)}$; but that leads to a broader scheme

$$\delta_m^{(2)} U_k^{(m)} = \left(\delta_k^{(1)} \right)^2 \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right), \quad (70)$$

which is apparently less attractive. This notice also applies to the next scheme.

The following scheme is based on Scheme 6.

Scheme 8 (New explicit scheme for (P2s)) *Let $\tilde{G}_{d,k}$ be what defined in (46), and corresponding discrete variational derivative in Lemma 13. Then for a given set of initial data $\mathbf{U}^{(0)}, \mathbf{V}^{(-\frac{1}{2})}, \mathbf{V}^{(\frac{1}{2})}$, we compute $\mathbf{U}^{(m)}, \mathbf{V}^{(m+\frac{1}{2})}$ ($m = 1, 2, \dots$) by*

$$\begin{aligned} \frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} &= \delta_k^+ \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} \right) \\ &= \delta_k^+ V_k^{(m+\frac{1}{2})}, \end{aligned} \quad (71a)$$

$$\frac{V_k^{(m+\frac{3}{2})} - V_k^{(m-\frac{1}{2})}}{2\Delta t} = \delta_k^- \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right), \quad (71b)$$

for $0 \leq k \leq N$.

Theorem 22 (Conservation property of Scheme 8) *Suppose that imposed discrete boundary conditions satisfy $B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) = 0$ ($m = 0, 1, 2, \dots$) and*

$$\begin{aligned} &\left[\left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \cdot s_k^+ \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} \right) \right. \\ &\left. + s_k^- \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} \right) \cdot \left(\frac{\delta \tilde{G}_d}{\delta(\mathbf{V}^{(m+\frac{3}{2})}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})_k} \right) \right]_0^N = 0. \end{aligned} \quad (72)$$

Then Scheme 6 is conservative in the sense

$$\sum_{k=0}^N {}''\tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{V}^{(m+\frac{1}{2})}, \mathbf{V}^{(m-\frac{1}{2})})\Delta x = \sum_{k=0}^N {}''\tilde{G}_{d,k}(\mathbf{U}^{(0)}, \mathbf{V}^{(\frac{1}{2})}, \mathbf{V}^{(-\frac{1}{2})})\Delta x, \quad (73)$$

for $m = 1, 2, \dots$, holds.

PROOF. The proof is similar to the previous theorem, except that this time the discrete variation identity in Lemma 13 is used. \square

In Section 2, it was noted that for the equations (P2), working with the system representation (P2s) is more convenient; this is still true in discrete context. It is surely possible to rewrite the above schemes into their reduced form by eliminating the intermediate variable \mathbf{V} so that only \mathbf{U} is used in the actual

computation. In the reduced schemes, however, we are forced to do a difficult task to calculate the discrete energy without using \mathbf{V} .

5 Applications

Application examples for the nonlinear Klein-Gordon equation (2) and the “good” Boussinesq equation (8) are presented. All the experiments were done with Windows PC system (CPU: Intel Pentium M 900MHz, 512MB memory) and Intel Fortran Compiler for Windows 8.0. To solve nonlinear system of equations, the numerical Newton solver NEQNF in IMSL, which provides very convenient way of implementing nonlinear schemes, is used.

5.1 Application to the nonlinear Klein-Gordon equation

Examples of conservative schemes in the literature for the nonlinear Klein-Gordon equation are [1,4,11,20,8]. Here four schemes are compared: the implicit Scheme 3, the explicit Scheme 4, the implicit scheme by Strauss[20], and the explicit scheme by Furihata[8]. The latter two were shown to be efficient and stable in Furihata[8].

The following numerical experiment is carried out following Furihata[8]. The function $\phi(u)$ is chosen to $-\cos(u)$, so that the equation becomes the sine-Gordon equation (SG):

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \sin u, \quad G(u, u_x) = \frac{u_x^2}{2} - \cos u. \quad (74)$$

The equation is considered over $x \in [-10, 10]$ under the Neumann boundary condition $u_x(-10, t) = u_x(10, t) = 0$. The SG has the exact solution

$$u(x, t) = 4 \arctan \left(\exp \left(\frac{x - ct}{\sqrt{1 - c^2}} \right) \right), \quad \text{where } c = 0.2, \quad (75)$$

when it is considered over the whole spatial domain $x \in (-\infty, \infty)$. This is truncated and used as the initial conditions for the numerical experiment. The discrete energy function in Scheme 3 is defined as

$$\tilde{G}_{d,k}(\mathbf{U}^{(m)}, \mathbf{V}^{(m)}) := \frac{1}{2} \left(\frac{(\delta_k^+ U_k^{(m)})^2 + (\delta_k^- U_k^{(m)})^2}{2} \right) - \cos(U_k^{(m)}) + \frac{(V_k^{(m)})^2}{2}. \quad (76)$$

The discrete partial derivatives becomes

$$\frac{\partial G_d}{\partial(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} = -\frac{\cos(U_k^{(m+1)}) - \cos(U_k^{(m)})}{U_k^{(m+1)} - U_k^{(m)}}, \quad (77a)$$

$$\frac{\partial G_d}{\partial \delta_k^\pm(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)})_k} = \delta_k^\pm \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right), \quad (77b)$$

$$\frac{\partial G_d}{\partial(\mathbf{V}^{(m+1)}, \mathbf{V}^{(m)})_k} = \frac{V_k^{(m+1)} + V_k^{(m)}}{2}. \quad (77c)$$

Then the concrete form of Scheme 3, which is addressed as the “new implicit scheme” below, becomes

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = \frac{V_k^{(m+1)} + V_k^{(m)}}{2}, \quad (78a)$$

$$\frac{V_k^{(m+1)} - V_k^{(m)}}{\Delta t} = \delta_k^{\langle 2 \rangle} \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right) + \frac{\cos(U_k^{(m+1)}) - \cos(U_k^{(m)})}{U_k^{(m+1)} - U_k^{(m)}}. \quad (78b)$$

The above scheme refers undefined points $U_{-1}^{(m)}, U_{N+1}^{(m)}$, which are resolved by the discrete Neumann boundary conditions,

$$U_{-1}^{(m)} = U_1^{(m)}, \quad U_{N+1}^{(m)} = U_N^{(m)}, \quad \text{for } m = 0, 1, 2, \dots \quad (79)$$

The assumption in Theorem 14 becomes

$$\begin{aligned} & B_1(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}) \\ &= \frac{1}{2} \left[\delta_k^+ \mu_m^+ U_k^{(m)} \cdot s_k^+ \delta_m^+ U_k^{(m)} + s_k^- \delta_k^+ \mu_m^+ U_k^{(m)} \cdot \delta_m^+ U_k^{(m)} \right. \\ & \quad \left. + \delta_k^- \mu_m^+ U_k^{(m)} \cdot s_k^- \delta_m^+ U_k^{(m)} + s_k^+ \delta_k^- \mu_m^+ U_k^{(m)} \cdot \delta_m^+ U_k^{(m)} \right]_0^N \\ &= \left[\delta_k^+ \mu_m^+ U_k^{(m)} \cdot \mu_k^+ \delta_m^+ U_k^{(m)} + \delta_k^- \mu_m^+ U_k^{(m)} \cdot \mu_k^- \delta_m^+ U_k^{(m)} \right]_0^N. \end{aligned} \quad (80)$$

In this calculation the trivial identities $s_k^- \delta_k^+ = \delta_k^-$, and $s_k^+ \delta_k^- = \delta_k^+$ are used. The right hand side vanishes in light of the discrete boundary conditions (79), which implies $\delta_k^+ \delta_m^+ U_k^{(m)} + \delta_k^- \delta_m^+ U_k^{(m)} = 0$ and $\mu_k^+ \delta_m^+ U_k^{(m)} - \mu_k^- \delta_m^+ U_k^{(m)} = 0$ at $k = 0, N$. Thus along the approximate solutions the discrete energy (76) remains constant. The discrete energy in Scheme 4 is defined by

$$\begin{aligned} & \tilde{G}_{d,k}(\mathbf{U}^{(m+1)}, \mathbf{U}^{(m)}, \mathbf{V}^{(m+1)}, \mathbf{V}^{(m)}) := \\ & \frac{1}{2} \left(\frac{(\delta_k^+ U_k^{(m+1)})(\delta_k^+ U_k^{(m)}) + (\delta_k^- U_k^{(m+1)})(\delta_k^- U_k^{(m)})}{2} \right) \\ & - \cos(\mu_m^+ U_k^{(m)}) + \frac{V_k^{(m+1)} V_k^{(m)}}{2}. \end{aligned} \quad (81)$$

Then the concrete form of Scheme 4, which is addressed as the “new explicit scheme” below, becomes

$$\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2\Delta t} = V_k^{(m)}, \quad (82a)$$

$$\frac{V_k^{(m+1)} - V_k^{(m-1)}}{2\Delta t} = \delta_k^{(2)} U_k^{(m)} + \frac{\cos(\mu_m^+ U_k^{(m)}) - \cos(\mu_m^- U_k^{(m)})}{\mu_m^+ U_k^{(m)} - \mu_m^- U_k^{(m)}}. \quad (82b)$$

The conservation property is confirmed similarly as above, from Theorem 15.

In each scheme, an attempt was made to find maximal time mesh size Δt beyond which the scheme became unstable. Table 1 shows the results, where N_t is the number of overall time steps. As to the maximal time mesh size in Strauss and Furihata schemes, the results in Furihata[8] are confirmed. The new explicit scheme only allows smaller time mesh sizes than Furihata’s explicit scheme; this is somewhat expected, since the scheme is “broader” than Furihata’s scheme (see (64)). In contrast to that, the new implicit scheme is surprisingly stable. Actually, it even integrates the problem only with *one* time step. Note that, the maximal time mesh size “20” just comes from the problem setting (the problem is integrated over $0 < t \leq 20$). With respect to the computation time, it is clear that explicit schemes are far faster than implicit schemes. The speed of Furihata’s explicit scheme, in particular, strikes us. The new explicit scheme falls behind it due to the restriction on the maximal time step size. The new implicit scheme is faster than Strauss’s scheme, thanks to its strong stability and wide time mesh size. Note that the computation times of implicit schemes strongly depends on the performance of the solver of nonlinear equations. They can be improved by optimizing the implementation.

Table 1

The SG: computation time and maximal time mesh size in each scheme

Scheme	Time (in seconds)	Max. Δt (N_t)
Strauss Implicit	0.100	0.5 (40)
Furihata Explicit	0.000350	0.8 (25)
New Implicit	0.0263	20 (1)
New Explicit	0.00128	0.25 (81)

Figure 1 shows the shapes of the numerical solutions. In each scheme, two results with different time mesh sizes around the maximal time mesh size are presented. That is, Strauss scheme with $N_t = 40, 38$; Furihata scheme with $N_t = 25, 20$; the new implicit scheme with $N_t = 5, 1$; and the new explicit scheme with $N_t = 81, 80$. The numerical solutions are plotted with fat circles, and the (untruncated) exact solution with solid surface. Except the new

implicit scheme, the schemes are shown to become unstable when the time mesh sizes exceed the limits. The vertical scales are fixed, so that the unstable solutions shortly jump out the screens.

Figure 2 shows the evolution of the discrete energies. The concrete forms of the discrete energies of Strauss[20] and Furihata[8] are summarized in Furihata[8]. As far as the time mesh sizes do not exceed the limit, the schemes happily conserve their corresponding discrete energies to the machine accuracy.

5.2 Application to the “good” Boussinesq equation

The “good” Boussinesq equation (GB) has quite peculiar soliton structures and have drawn much interests[12,13,6,22]. To summarize, solitons behave in completely different ways depending on their amplitudes. For example, the GB has the one soliton solution on the whole interval $x \in (-\infty, \infty)$:

$$u(x, t) = -A \operatorname{sech}^2 \left(\frac{p}{2}(x - ct) \right), \quad (83)$$

where $A > 0$ is “amplitude,” $p = \sqrt{2A/3}$, and $c = \sqrt{1 - 2A/3}$. Observe that the velocity c becomes imaginary for $A > 3/2$. In that region the soliton ceases to exist; i.e. the GB admits the soliton solution only for a finite range of velocity. The more interesting phenomena is observed when two solitons collide; if both solitons are small enough, they pass through each other like as the other usual solitons do. But when they exceed some limit, the solution “blows-up” at the collision, even if both amplitudes are smaller than $3/2$ for being stable one-solitons.

Another noteworthy feature of the GB is that it can be formulated as a Hamiltonian system[21,19], and in view of this, several numerical schemes were developed[5,3]. Strangely, however, no conservative scheme have been explicitly considered so far. One reason for this may be that in general no scheme can be both symplectic and Hamiltonian-conserving[9], and for Hamiltonian systems, symplectic integrators have drawn more attention in these years than Hamiltonian-conserving integrators, though it is still not clear in PDE contexts which approach is better. In this paper, we focus our attention on Hamiltonian-conserving schemes. The GB is considered over $x \in [-75, 75]$, and u, u_x, u_{xx}, v, v_x are assumed to be periodic in space. As the initial data, the soliton solution above is truncated and used. The missing initial value $v(x, 0)$ is obtained as $v(x, 0) = \int_{-75}^x u_t(x, 0)dx = -cu(x, 0)$, if we neglect the exponentially small boundary value $u_t(-75, 0)$. In all the experiments below, the number of spatial mesh points are taken to $N = 200$.

Two conservative schemes are presented and tested below. The first, addressed

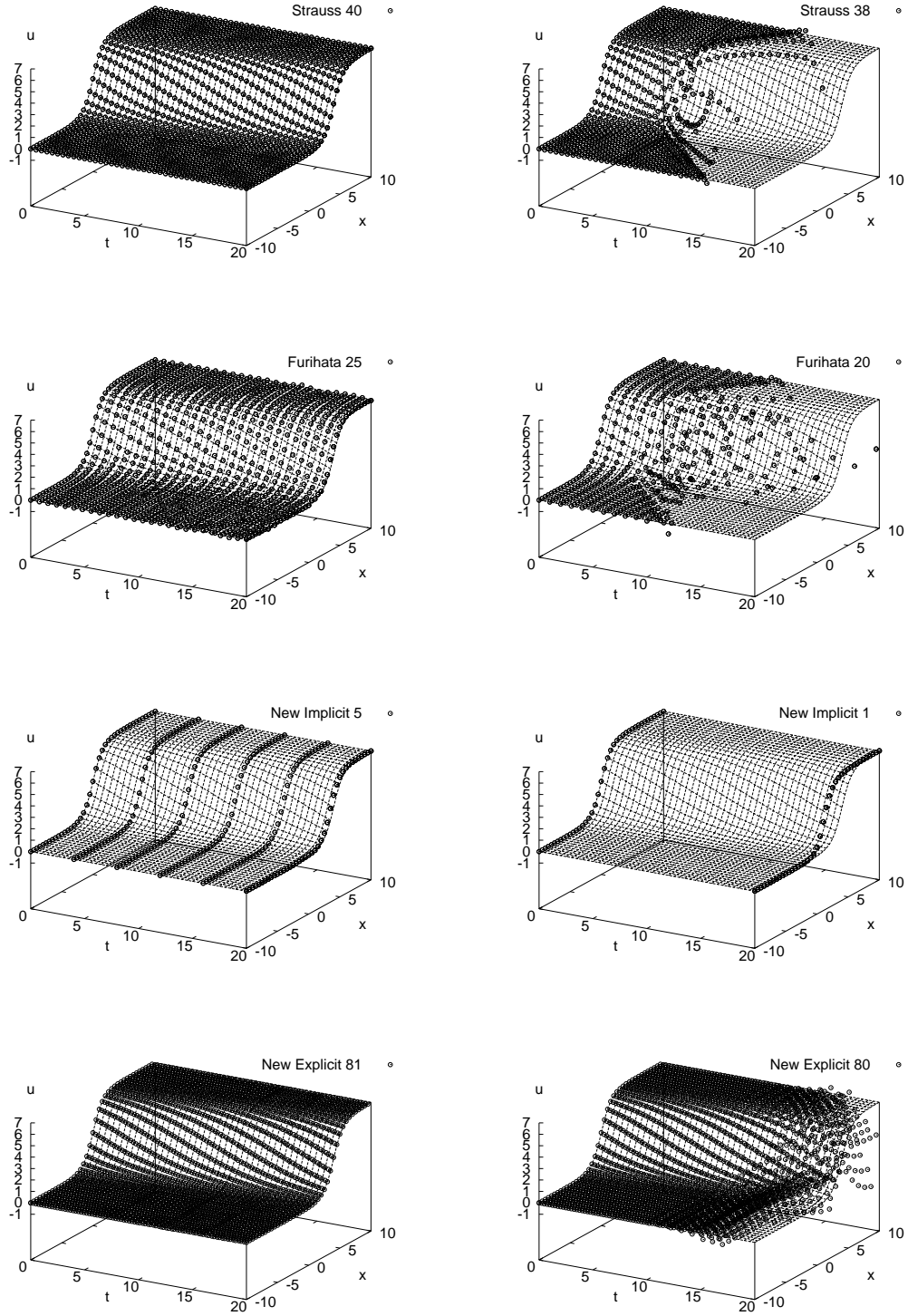


Fig. 1. The SG: numerical solutions; (top) Strauss Implicit $N = 40, 38$, (middle upper) Furihata Explicit $N = 25, 20$, (middle lower) New Implicit $N = 5, 1$, (bottom) New Explicit $N = 81, 80$

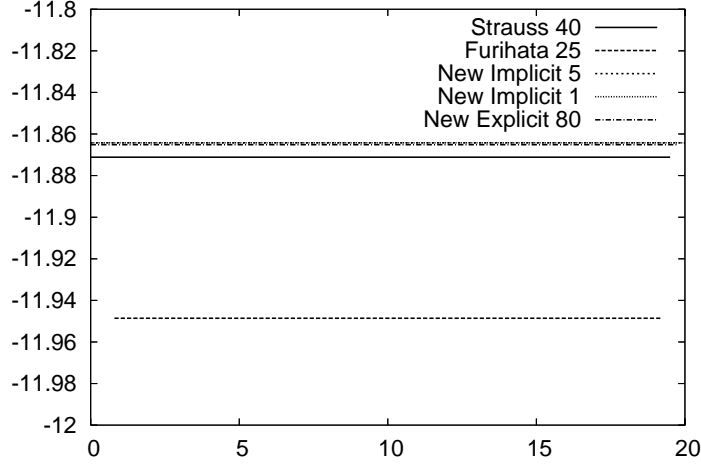


Fig. 2. The SG: evolutions of the discrete energies

as the “implicit scheme,” is Scheme 7 with

$$\tilde{G}_{d,k} := \frac{(U_k^{(m)})^2}{2} + \frac{(U_k^{(m)})^3}{3} + \frac{(\delta_k^+ U_k^{(m)})^2 + (\delta_k^- U_k^{(m)})^2}{4} + \frac{(V_k^{(m)})^2}{2}, \quad (84)$$

whose concrete form becomes

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = \delta_k^+ \left(\frac{V_k^{(m+1)} + V_k^{(m)}}{2} \right), \quad (85a)$$

$$\begin{aligned} \frac{V_k^{(m+1)} - V_k^{(m)}}{\Delta t} = & \delta_k^- \left(\mu_m^+ U_k^{(m)} - \delta_k^{(2)} \mu_m^+ U_k^{(m)} \right. \\ & \left. + \frac{(U_k^{(m+1)})^2 + U_k^{(m+1)} U_k^{(m)} + (U_k^{(m)})^2}{3} \right). \end{aligned} \quad (85b)$$

The references outside $0 \leq k \leq N$ are resolved with the discrete periodic boundary conditions

$$U_k^{(m)} = U_{(k+N) \bmod N}^{(m)} \quad \text{and} \quad V_k^{(m)} = V_{(k+N) \bmod N}^{(m)}, \quad \text{for } m = 0, 1, 2, \dots \quad (86)$$

Under these conditions, the assumptions in Theorem 21 are satisfied, and the conservation property holds. The second one is Scheme 8 with

$$\tilde{G}_{d,k} := \frac{(U_k^{(m)})^2}{2} + \frac{(U_k^{(m)})^3}{3} + \frac{(\delta_k^+ U_k^{(m)})^2 + (\delta_k^- U_k^{(m)})^2}{4} + \frac{V_k^{(m+\frac{1}{2})} V_k^{(m-\frac{1}{2})}}{2}, \quad (87)$$

whose concrete form becomes

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = \delta_k^+ V_k^{(m+\frac{1}{2})}, \quad (88a)$$

$$\begin{aligned} \frac{V_k^{(m+\frac{3}{2})} - V_k^{(m-\frac{1}{2})}}{2\Delta t} = & \delta_k^- \left(\mu_m^+ U_k^{(m)} - \delta_k^{(2)} \mu_m^+ U_k^{(m)} \right. \\ & \left. + \frac{(U_k^{(m+1)})^2 + U_k^{(m+1)} U_k^{(m)} + (U_k^{(m)})^2}{3} \right). \end{aligned} \quad (88b)$$

The scheme is called the “explicit scheme” below.

Firstly, the computation times and maximal time mesh size allowed in each scheme are examined. The amplitude is taken to $A = 0.5$ (accordingly $p \simeq 0.55735$, $c = 0.81650$). Then the problem is integrated over $0 \leq t \leq 40$. Table 2 summarizes the results. The implicit scheme can integrate the problem with only one time step, and thus is quite stable. In the explicit scheme, there is a restriction on the size of time mesh; but thanks to being explicit, it is quite fast. In each scheme the discrete energy is conserved to the machine accuracy (the graph is omitted).

Table 2

The GB: computation time and maximal time mesh size in each scheme

Scheme	Time (in seconds)	Max. Δt (N_t)
New Implicit	1.10	40 (1)
New Explicit	0.0338	0.263 (152)

Secondly, long-time behaviours of the schemes are verified. The truncated one soliton solution ($A = 0.5$) is integrated over very long time $0 \leq t \leq 10000$, in which the soliton goes around the spatial interval about 184 times. In the implicit scheme $N_t = 10000$ ($\Delta t = 1$), and in the explicit scheme $N_t = 40000$ ($\Delta t = 1/4$). Figure 3 shows the results, where only 100 snap shots are drawn to avoid the screens being painted out. In both graphs, the soliton solution successfully propagates keeping its soliton shape. Figure 4 shows the evolutions of the discrete energies. Both are well conserved; actually they are conserved up to the machine accuracy.

Thirdly, more qualitative aspects of the schemes are explored. To this end, the collision of two small solitons is considered; namely, the initial conditions are set to $u(x, 0) = \phi_c(x + 50, 0) + \phi_{-c}(x - 50, 0)$, and $u_t(x, 0) = -c\phi_c(x + 50, 0) + c\phi_{-c}(x - 50, 0)$, where $\phi_c(x, t)$ is the one-soliton solution (83), and $\phi_{-c}(x, t)$ is its flipped version with the velocity $-c$. The size of velocities of the two solitons (and accordingly the amplitudes) are set to equal. Two cases with different amplitudes $A = 0.3$ and $A = 0.4$ are experimented. In [12] it was reported that the solution blew up numerically when $A > 0.3691$. In this experiment, the number of temporal mesh points are taken to $N_t = 100$

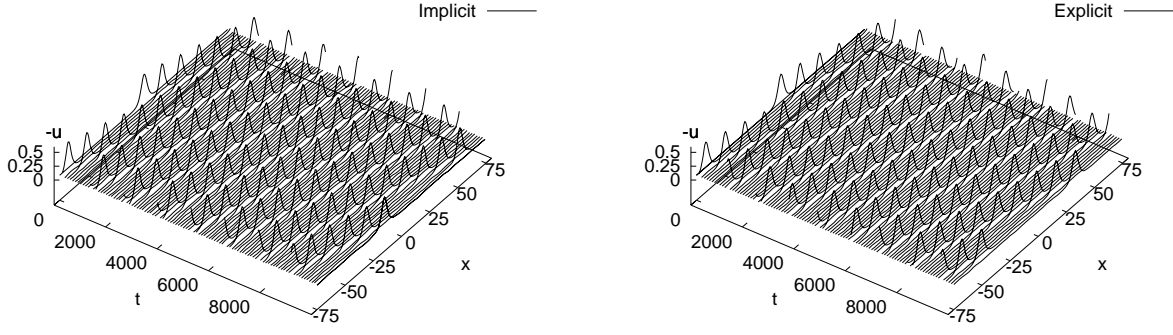


Fig. 3. The GB: numerical one solitons; (left) Implicit scheme $N_t = 10000$, (right) Explicit scheme $N_t = 40000$

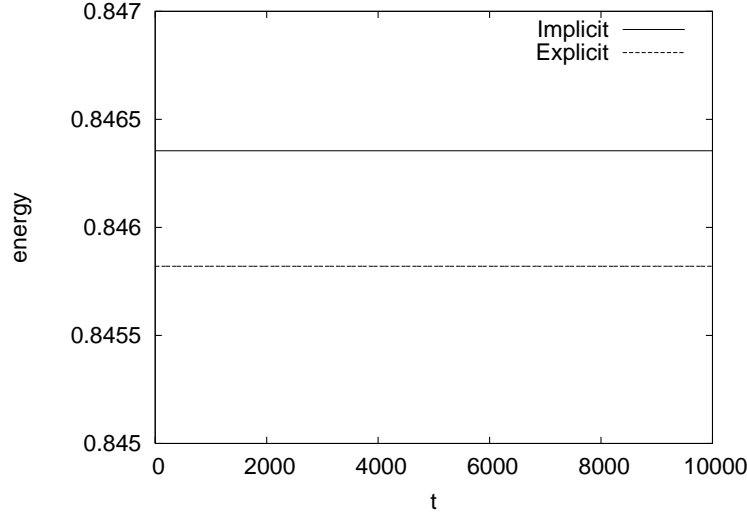


Fig. 4. The GB: evolutions of the discrete energies (one soliton case)

in the implicit scheme, and $N_t = 400$ in the explicit scheme, and the problem is integrated over $0 \leq t \leq 100$. Figure 5 shows the results. When $A = 0.3$, both the implicit and explicit schemes successfully track the collision of the solitons. When $A = 0.4$, however, the situation dramatically changes. Both graphs suddenly end around $t \sim 60$. In the implicit scheme, the Newton solver fails to find the solution there. In the explicit scheme, the solution becomes fairly unstable and is destroyed (the solution jump out the screen there). This agrees with the blow-up result in [12]. In Figure 6 are the conservation results. When $A = 0.3$, the discrete energies are conserved to the machine accuracy. When $A = 0.4$, they are conserved for a short while, but collapse at around $t \sim 60$ due to the blow-up of the solution.

Remark 23 In this paper, only the lowest order spatial difference operators are considered for simplicity. The order can be arbitrarily increased under the

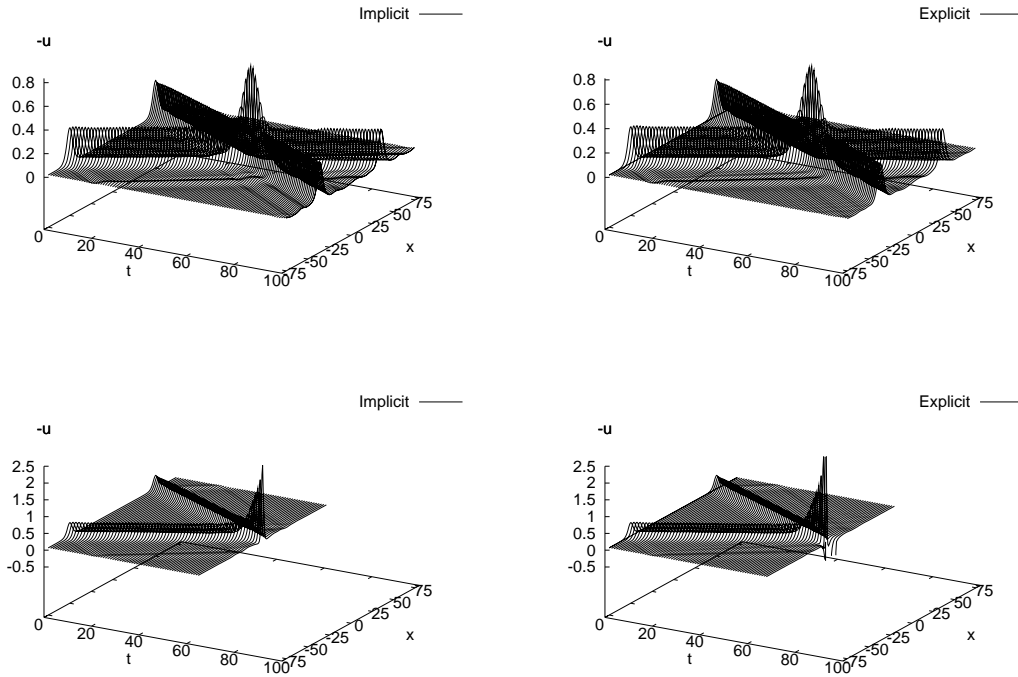


Fig. 5. The GB: numerical two solitons; (top left) implicit, $A = 0.3$, (top right) explicit, $A = 0.3$, (bottom left) implicit, $A = 0.4$, (bottom right) explicit, $A = 0.4$

discrete periodic boundary condition, using the technique developed in [18]. In particular, conservative pseudospectral schemes can be derived which seem to be promising.

6 Concluding remarks

In this paper a new approach for designing conservative schemes for the non-linear wave equations, (P1) and (P2), is proposed. The essential idea there is to employ the system representations (P1s) and (P2s), and develop the multi-variate versions of discrete variational derivatives. Several new schemes based on this approach are presented, and the relation between this new approach and the previous approach is clarified. To summarize, the new approach has the following advantages: (a) it can provide further stabler schemes; (b) it includes the previous approach in that the previous schemes can also be derived out of the new approach; (c) in some new schemes, the time mesh can be adaptively changed; and (d) the equations (P2) is covered for the first time in the new approach. Numerical experiments for the Sine-Gordon equation and the “good” Boussinesq (GB) equation are presented, which confirm the usefulness of the proposed approach. For the GB, in particular, the schemes

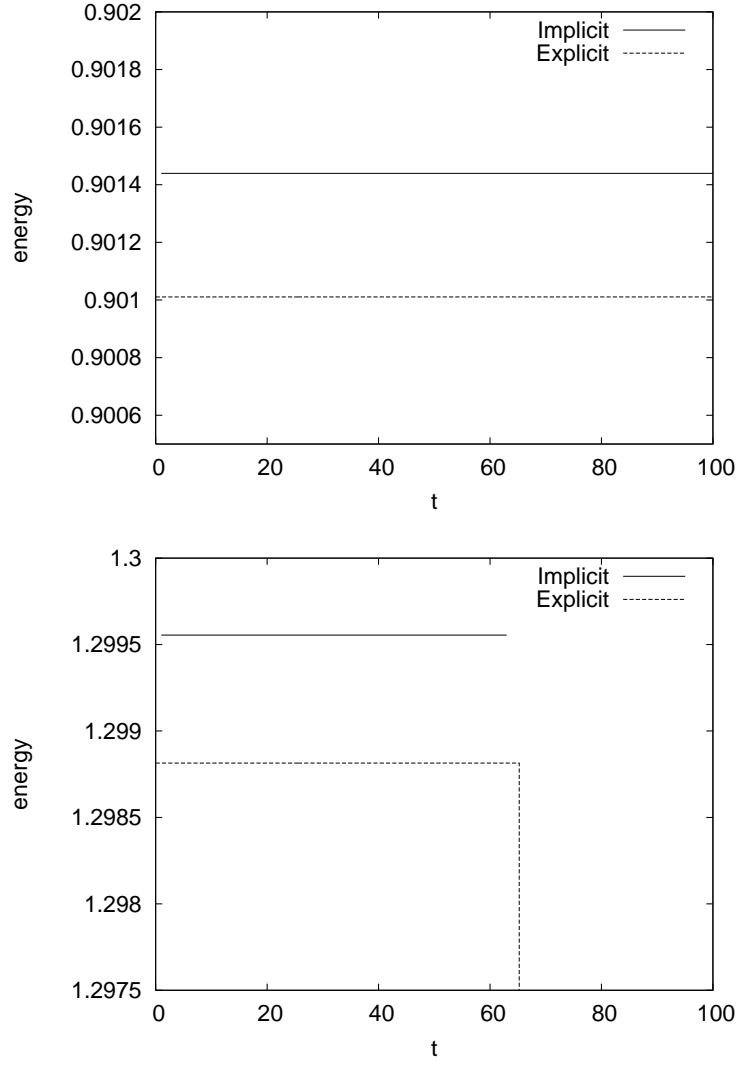


Fig. 6. The GB: evolutions of the discrete energies (two soliton case); (top) $A = 0.3$, (bottom) $A = 0.4$

in this paper seem to be the first conservative schemes in the literature as far as the author knows.

The remaining issues include the followings. First, for the wave equations the symplectic, particularly the multi-symplectic integrators[10] are also promising. Careful comparisons between these integrators and the present approach should be made both theoretically and numerically. Second, high-order versions of the presented schemes, which can be constructed using the techniques in [14,18,15,16], should be tested. The author is now working on this issue, and the report will be reported as soon as it is possible.

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