Multi-Symplectic Runge-Kutta Collocation Methods for Hamiltonian Wave Equations

Sebastian Reich
Department of Mathematics and Statistics
University of Surrey, Guildford, GU2 5XH

August 25, 1999

Abstract

A number of conservative PDEs, like various wave equations, allow for a multi-symplectic formulation which can be viewed as a generalization of the symplectic structure of Hamiltonian ODEs. We show that Gauss-Legendre collocation in space and time leads to multi-symplectic integrators, i.e., to numerical methods that preserve a symplectic conservation law similar to the conservation of symplecticity under a symplectic method for Hamiltonian ODEs. We also discuss the issue of conservation of energy and momentum. Since time discretization by a Gauss-Legendre method is computational rather expensive, we suggest several semi-explicit multi-symplectic methods based on Gauss-Legendre collocation in space and explicit or linearly implicit symplectic discretizations in time.

1 Introduction

The scalar wave equation

$$\partial_{tt} u = \partial_{xx} u - V'(u), \quad (x,t) \in \mathcal{U} \subset \mathbb{R}^2, \tag{1}$$

$V : \mathbb{R} \to \mathbb{R}$ some smooth function, is an example of a multi-symplectic Hamiltonian PDE [3] of type

$$\mathbf{M}\partial_t \boldsymbol{z} + \mathbf{K}\partial_x \boldsymbol{z} = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}) \tag{2}$$

where $\boldsymbol{z} \in \mathbb{R}^d$, $\mathbf{M}, \mathbf{K} \in \mathbb{R}^{d\times d}$ are two skew-symmetric matrices (which can be singular), and $S : \mathbb{R}^d \to \mathbb{R}$ is a smooth function. In the particular case of the wave equation (1), a multi-symplectic formulation (2) can be derived as follows [3]. We introduce canonical momenta $v = \partial_t u$, $w = \partial_x u$ and define the state variable

$$\boldsymbol{z} = \begin{bmatrix} u \\ v \\ w \end{bmatrix} \in \mathbb{R}^3.$$

Using this variable, we obtain

$$\mathbf{M} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{K} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

as well as the Hamiltonian

$$S(\boldsymbol{z}) = \frac{1}{2}\left(v^2 - w^2\right) + V(u).$$

Other Hamiltonian PDEs that can be rewritten as a multi-symplectic system (2) include the nonlinear Schrödinger equation (see §6), the Boussinesq equation, the shallow water equation, and the Korteweg-de Vries equation [3, 4, 5].

The multi-symplectic reformulation (2) is interesting for several reasons (see [3, 4, 5] for theoretical results), one of the most important perhaps being the existence of the multi-symplectic conservation law

$$\partial_t [\boldsymbol{dz} \wedge \mathbf{M}\boldsymbol{dz}] + \partial_x [\boldsymbol{dz} \wedge \mathbf{K}\boldsymbol{dz}] = 0 \tag{3}$$

which, for the wave equation (1), is equivalent to

$$\partial_t [\boldsymbol{du} \wedge \boldsymbol{dv}] - \partial_x [\boldsymbol{du} \wedge \boldsymbol{dw}] = 0. \tag{4}$$

In other words, changes in the wedge product $\boldsymbol{du} \wedge \boldsymbol{dv}$ in time are exactly compensated for by changes in the wedge product $\boldsymbol{du} \wedge \boldsymbol{dw}$ in space. We note that this is a strictly local conservation concept that, e.g., does not depend on specific boundary conditions. This is in contrast to the classical formulation of the wave equation (1) as a Hamiltonian initial value problem over some appropriate function space. Furthermore, for conservative systems that do not depend on a spatial direction (like Newton's equations of motion), we obtain the classical result

$$\frac{d}{dt} [\boldsymbol{du} \wedge \boldsymbol{dv}] = \frac{d}{dt} \sum_{k=1}^{M} \boldsymbol{du}_k \wedge \boldsymbol{dv}_k = 0$$

where $\boldsymbol{u} \in \mathbb{R}^M$ would be the vector of coordinates and $\boldsymbol{v} \in \mathbb{R}^M$ the vector of canonical momenta.

It is widely recognised that the symplectic structure of phase space should be taken into account when it comes to numerical simulations of Hamiltonian systems. In particular, methods that preserve the wedge product $\boldsymbol{du} \wedge \boldsymbol{dv}$ exist for canonical (finite-dimensional) Hamiltonian systems and are called symplectic methods [18]. A discussion of symplectic methods for finite dimensional spatial truncations of the wave equation (1) can be found, for example, in [13, 8]. The basic idea is to find a finite dimensional spatial truncation

$$\frac{d}{dt}\boldsymbol{u} = \boldsymbol{v}, \tag{5}$$

$$\frac{d}{dt}\boldsymbol{v} = \boldsymbol{A}\boldsymbol{u} - \boldsymbol{V}'(\boldsymbol{u}) \tag{6}$$

$\boldsymbol{u} = (u_1, \ldots, u_M)^T$, $\boldsymbol{v} = (v_1, \ldots, v_M)^T$ where $\boldsymbol{A} \in \mathbb{R}^{M\times M}$ is a finite-difference approximation to ∂_{xx} and $\boldsymbol{V}'(\boldsymbol{u}) = (V'(u_1), V'(u_2), \ldots, V'(u_M))^T$, M the number of grid points. This differential equation (5)-(6) is Hamiltonian in the variable $(\boldsymbol{u}, \boldsymbol{v}) \in \mathbb{R}^{2M}$ if $\boldsymbol{A}$ is symmetric leading to the invariance of the symplectic structure $\boldsymbol{du} \wedge \boldsymbol{dv}$. Typically $\boldsymbol{A}$ is obtained using the second central difference approximation (leapfrog) but higher order symmetric finite difference approximations are also occasionally applied [8]. This system (5)-(6) can now be integrated in time using a symplectic discretization. For example, if $\boldsymbol{A}$ is the second central difference approximation and (5)-(6) is discretized by the Störmer-Verlet method [18], then the popular leapfrog discretization of the nonlinear wave equation (1) is obtained. Instead of applying a symplectic discretization in time one can also use an energy conserving discretization. This option has, for example, been explored in [19, 10, 15].

Contrary to this "classical" approach, the investigation of multi-symplectic numerical methods for Hamiltonian PDEs is a very recent subject. The first paper is due to Marsden, Patrick & Shkoller [11] who used a formulation of the multi-symplectic structure for wave equations based on a Lagrangian formulation of the Cartan form in field theory [12]. They then derive a numerical scheme by discretizing the Lagrangian. This leads to an elegant generalization of Veselov discretizations [20] to PDEs. However, there are limitations in a Lagrangian setting, such as restrictions on the order of numerical discretizations. A new definition of multi-symplectic integrators based on a discrete form of the symplectic conservation law (3) was recently suggested by BRIDGES & REICH in [6]. It has been shown that popular methods such as the centered Preissmann scheme [1] and the leapfrog method are multi-symplectic and that such schemes have remarkable local energy and momentum conserving properties [6].

In this paper, we like to explore the question of whether or not symplectic methods

$$\boldsymbol{z}^{n+1} = \boldsymbol{\psi}_{\Delta t}(\boldsymbol{z}^n), \qquad t_{n+1} = t_n + \Delta t,$$

for canonical Hamiltonian ODEs

$$\frac{d}{dt}\boldsymbol{z} = \mathbf{J}^{-1}\boldsymbol{\nabla}_{\boldsymbol{z}} H(\boldsymbol{z}), \quad \boldsymbol{z} \in \mathbb{R}^{2M}, \; \mathbf{J} = -\mathbf{J}^T, \tag{7}$$

with their exact conservation property

$$\boldsymbol{d}\boldsymbol{z}^{n+1} \wedge \mathbf{J}\boldsymbol{d}\boldsymbol{z}^{n+1} = \boldsymbol{d}\boldsymbol{z}^n \wedge \mathbf{J}\boldsymbol{d}\boldsymbol{z}^n$$

can be generalised to multi-symplectic PDEs (2). The main objective is to formulate higher order multi-symplectic discretizations. For simplicity of exposition, we will restrict to the nonlinear wave equation (1) and one of our main results is that we show that a proper implementation of Gauss-Legendre collocation methods [18] leads to a multi-symplectic numerical scheme for (1). See §6 for a brief discussion of the non-linear Schrödinger equation. We point out that the spatial discretization by Gauss-Legendre collocation methods leads to a particular type of the pseudospectral (cell) methods [9]. It is known that these methods are well suited for the integration of very smooth solutions over long periods of time under a stringent error requirement [9].

One of the main justifications for applying symplectic methods to (finite-dimensional) Hamiltonian systems (7) stems from their excellent conservation of the Hamiltonian (energy) H over very long integration intervals $t_n \in [0, T]$ [2]. For a multi-symplectic system (2), conservation of energy is replaced by the following local conservation law [4]:

$$\partial_t E(\boldsymbol{z}) + \partial_x F(\boldsymbol{z}) = 0. \tag{8}$$

The energy density is

$$E(\boldsymbol{z}) = S(\boldsymbol{z}) - \frac{1}{2}\boldsymbol{z}^T\mathbf{K}\partial_x\boldsymbol{z}$$

and the energy flux is

$$F(\boldsymbol{z}) = \frac{1}{2}\boldsymbol{z}^T\mathbf{K}\partial_t\boldsymbol{z}.$$

This can be seen from

$$0 = \partial_t\boldsymbol{z}^T\mathbf{M}\partial_t\boldsymbol{z} = \partial_t S(\boldsymbol{z}) - \partial_t\boldsymbol{z}^T\mathbf{K}\partial_x\boldsymbol{z} = \partial_t S(\boldsymbol{z}) - \frac{1}{2}\partial_t[\boldsymbol{z}^T\mathbf{K}\partial_x\boldsymbol{z}] + \frac{1}{2}\partial_x[\boldsymbol{z}^T\mathbf{K}\partial_t\boldsymbol{z}].$$

For the wave equation (1), we can eliminate the partial derivatives in E and F and can formulate an energy conservation law (8) with

$$E = \frac{1}{2}\left(w^2 + v^2\right) + V(u) \quad \text{and} \quad F = -vw$$

where we have made use of the identity $\partial_x v = \partial_t w = \partial_{tx} u$. There is a corresponding momentum conservation law which is obtained by premultiplying (2) by $\partial_x\boldsymbol{z}^T$ [4]. For the wave equation, we can again simplify the corresponding expressions and obtain a momentum conservation law

$$\partial_t I(\boldsymbol{z}) + \partial_x G(\boldsymbol{z}) = 0 \tag{9}$$

with

$$I(\boldsymbol{z}) = F(\boldsymbol{z}) = -vw \qquad \text{and} \qquad G(\boldsymbol{z}) = \frac{1}{2}\left(w^2 + v^2\right) - V(u).$$

It is known that Gauss-Legendre methods exactly preserve quadratic first integrals of ordinary differential equations [7, 18]. One could therefore expect that a Gauss-Legendre discretization of the wave equation (1) leads to a discrete energy/momentum conservation law if the function V is zero or at most quadratic in u. As we will see in §3, this analogy does indeed hold.

2 Gauss-Legendre Discretizations are Multi-Symplectic

Let us state the multi-symplectic formulation of the wave equation (1) in the form

$$\partial_t u = v, \tag{10}$$

$$\partial_x u = w, \tag{11}$$

$$\partial_t v - \partial_x w = -V'(u). \tag{12}$$

The corresponding equations for the differential one forms $\boldsymbol{dz} = (\boldsymbol{du}, \boldsymbol{dv}, \boldsymbol{dw})^T$ are given by

$$\begin{aligned}
\partial_t \boldsymbol{du} &= \boldsymbol{dv}, \\
\partial_x \boldsymbol{du} &= \boldsymbol{dw}, \\
\partial_t \boldsymbol{dv} - \partial_x \boldsymbol{dw} &= -V''(u)\boldsymbol{du}.
\end{aligned}$$

This yields the multi-symplectic conservation law (4) via

$$\boldsymbol{du} \wedge \partial_t \boldsymbol{dv} - \boldsymbol{du} \wedge \partial_x \boldsymbol{dw} = -V''(u)\boldsymbol{du} \wedge \boldsymbol{du} = 0$$

together with the observation that

$$\partial_t \left[\boldsymbol{du} \wedge \boldsymbol{dv}\right] = \partial_t \boldsymbol{du} \wedge \boldsymbol{dv} + \boldsymbol{du} \wedge \partial_t \boldsymbol{dv} = \boldsymbol{dv} \wedge \boldsymbol{dv} + \boldsymbol{du} \wedge \partial_t \boldsymbol{dv} = \boldsymbol{du} \wedge \partial_t \boldsymbol{dv}$$

and, similarly,

$$\partial_x \left[\boldsymbol{du} \wedge \boldsymbol{dw}\right] = \boldsymbol{du} \wedge \partial_x \boldsymbol{dw}.$$

Let us now discretize (10)-(12) by a Gauss-Legendre collocation method written in the form of an implicit Runge-Kutta method [18]. We start with the spatial discretization and rewrite (10)-(12) as

$$\partial_x u = w, \tag{13}$$

$$\partial_x w = \partial_t v + V'(u), \tag{14}$$

$$0 = \partial_t u - v \tag{15}$$

Next we apply an implicit Runge-Kutta (RK) scheme with s stage variables (U_i, W_i) and coefficients $\{a_{ij}\}$, $\{b_i\}$ to (13)-(14) and obtain the semi-discretization

$$U_i = u_k + \Delta x \sum_{j=1}^{s} a_{ij} W_j, \tag{16}$$

$$W_i = w_k + \Delta x \sum_{j=1}^{s} a_{ij} \left(\partial_t V_j + V'(U_j)\right), \tag{17}$$

$$u_{k+1} = u_k + \Delta x \sum_{i=1}^{s} b_i W_i, \tag{18}$$

$$w_{k+1} = w_k + \Delta x \sum_{i=1}^{s} b_i \left(\partial_t V_i + V'(U_i)\right) \tag{19}$$

which is defined for all t. Note that $u_k(t)$ is an approximation to $u(x_k,t)$. For simplicity, we set $k=0$ and assume that $x_k=0$.

Let us check if this semi-discretization of the wave equation (2) implies a corresponding semi-discretized version of the conservation law (4). We first derive the equations for the differentials

$$\boldsymbol{d}U_i = \boldsymbol{d}u_0 + \Delta x \sum_{j=1}^{s} a_{ij}\boldsymbol{d}W_j, \tag{20}$$

$$\boldsymbol{d}W_i = \boldsymbol{d}w_0 + \Delta x \sum_{j=1}^{s} a_{ij}\left(\partial_t \boldsymbol{d}V_j + V''\boldsymbol{d}U_j\right), \tag{21}$$

$$\boldsymbol{d}u_1 = \boldsymbol{d}u_0 + \Delta x \sum_{i=1}^{s} b_i\boldsymbol{d}W_i, \tag{22}$$

$$\boldsymbol{d}w_1 = \boldsymbol{d}w_0 + \Delta x \sum_{i=1}^{s} b_i\left(\partial_t \boldsymbol{d}V_i + V''\boldsymbol{d}U_i\right). \tag{23}$$

Using (22) and (23), we proceed with

$$\begin{aligned}
\boldsymbol{d}u_1\wedge\boldsymbol{d}w_1 &= \left(\boldsymbol{d}u_0 + \Delta x \sum_{i=1}^{s} b_i\boldsymbol{d}W_i\right)\wedge\left(\boldsymbol{d}w_0 + \Delta x \sum_{i=1}^{s} b_i\left(\partial_t \boldsymbol{d}V_i + V''\boldsymbol{d}U_i\right)\right)\\
&= \boldsymbol{d}u_0\wedge\boldsymbol{d}w_0 + \boldsymbol{d}u_0\wedge\Delta x \sum_{i=1}^{s} b_i\left(\partial_t \boldsymbol{d}V_i + V''\boldsymbol{d}U_i\right) + \Delta x \sum_{i=1}^{s} b_i\boldsymbol{d}W_i\wedge\boldsymbol{d}w_0 +\\
&\quad + \Delta x^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i b_j \boldsymbol{d}W_i\wedge\left(\partial_t \boldsymbol{d}V_j + V''\boldsymbol{d}U_j\right).
\end{aligned}$$

This is further transformed to

$$\begin{aligned}
\boldsymbol{d}u_1\wedge\boldsymbol{d}w_1 &= \boldsymbol{d}u_0\wedge\boldsymbol{d}w_0 + \Delta x \sum_{i=1}^{s} b_i\boldsymbol{d}U_i\wedge\partial_t\boldsymbol{d}V_i +\\
&\quad + \Delta x^2 \sum_{i=1}^{s}\sum_{j=1}^{s}\left(b_ib_j - b_ja_{ji} - b_ia_{ij}\right)\boldsymbol{d}W_i\wedge\left(\partial_t \boldsymbol{d}V_j + V''\boldsymbol{d}U_j\right)
\end{aligned}$$

using (20)-(21). The last term is zero for Gauss-Legendre methods since [18]

$$b_ja_{ji} + b_ia_{ij} - b_ib_j = 0$$

for all i,j. Thus, upon applying a Gauss-Legendre RK method, we obtain the semi-discretized conservation law

$$\left[\boldsymbol{d}u_1\wedge\boldsymbol{d}w_1 - \boldsymbol{d}u_0\wedge\boldsymbol{d}w_0\right] - \sum_{i=1}^{s} b_i\left[\boldsymbol{d}U_i\wedge\partial_t\boldsymbol{d}V_i\right]\Delta x = 0 \tag{24}$$

which holds for all t.

The next step is the discretization in time over a time interval $[0,\Delta t]$. Since we are using an implicit RK methods, we can solve (16)-(17) for $\partial_t V_j(t)$, $j=1,\ldots,s$. We also use equation (15) and implement a Runge-Kutta time-discretization with r stages and coefficients $\{\tilde{a}_{mn}\}$, $\{\tilde{b}_m\}$:

$$U_{i,m} = u_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn}V_{i,n}, \tag{25}$$

$$
\begin{aligned}
V_{i,m} &= v_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t V_{i,n}, && (26)\\
u_i^1 &= u_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m V_{i,m}, && (27)\\
v_i^1 &= v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t V_{i,m}. && (28)
\end{aligned}
$$

Here we introduced the notation

$$
U_{i,m} \approx u(c_i \Delta x, d_m \Delta t), \quad u_i^1 \approx u(c_i \Delta x, \Delta t), \quad u_1^m \approx u(\Delta x, d_m \Delta t)
$$

etc. with

$$
c_i = \sum_{j=1}^{s} a_{ij} \qquad \text{and} \qquad d_m = \sum_{n=1}^{r} \tilde{a}_{mn}.
$$

The symbol $\partial_t V_{i,m}$ denotes the numerical approximation of $\partial_t V_i(d_m \Delta t)$ which we obtain from (16)-(17) by fixing $t = d_m \Delta t$.

Now we assume again that a Gauss-Legendre method is used and, upon applying similar arguments as before, we obtain the identity

$$
\begin{aligned}
\boldsymbol{d}u_i^1 \wedge \boldsymbol{d}v_i^1 &= \left(\boldsymbol{d}u_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \boldsymbol{d}V_{i,m} \right) \wedge \left(\boldsymbol{d}v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t \boldsymbol{d}V_{i,m} \right)\\
&= \boldsymbol{d}u_i^0 \wedge \boldsymbol{d}v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \boldsymbol{d}U_{i,m} \wedge \partial_t \boldsymbol{d}V_{i,m}
\end{aligned}
$$

or

$$
\left[\boldsymbol{d}u_i^1 \wedge \boldsymbol{d}v_i^1 - \boldsymbol{d}u_i^0 \wedge \boldsymbol{d}v_i^0 \right] - \sum_{m=1}^{r} \tilde{b}_m \left[\boldsymbol{d}U_{i,m} \wedge \partial_t \boldsymbol{d}V_{i,m} \right] \Delta t = 0.
$$

Next we rewrite (24) for $t = d_m \Delta t$ as

$$
\left[\boldsymbol{d}u_1^m \wedge \boldsymbol{d}w_1^m - \boldsymbol{d}u_0^m \wedge \boldsymbol{d}w_0^m \right] - \sum_{i=1}^{s} b_i \left[\boldsymbol{d}U_{i,m} \wedge \partial_t \boldsymbol{d}V_{i,m} \right] \Delta x = 0
$$

and obtain the discretized conservation law

$$
\sum_{i=1}^{s} b_i \left[\boldsymbol{d}u_i^1 \wedge \boldsymbol{d}v_i^1 - \boldsymbol{d}u_i^0 \wedge \boldsymbol{d}v_i^0 \right] \Delta x - \sum_{m=1}^{r} \tilde{b}_m \left[\boldsymbol{d}u_1^m \wedge \boldsymbol{d}w_1^m - \boldsymbol{d}u_0^m \wedge \boldsymbol{d}w_0^m \right] \Delta t = 0 \qquad (29)
$$

This formula can be understood as the approximation of the integral of (4) over the domain of integration $[0, \Delta x] \times [0, \Delta t]$, i.e., (29) approximates

$$
\begin{aligned}
&\int_{x=0}^{\Delta x} \left[\boldsymbol{d}u(x, \Delta t) \wedge \boldsymbol{d}v(x, \Delta t) - \boldsymbol{d}u(x, 0) \wedge \boldsymbol{d}v(x, 0) \right] dx \; - \\
&\qquad - \int_{t=0}^{\Delta t} \left[\boldsymbol{d}u(\Delta x, t) \wedge \boldsymbol{d}w(\Delta x, t) - \boldsymbol{d}u(0, t) \wedge \boldsymbol{d}w(0, t) \right] dt \;=\; 0 \qquad (30)
\end{aligned}
$$

using Gaussian quadrature for the evaluation of the two integrals.

Proposition 1. Let the multi-symplectic formulation (10)-(12) of the nonlinear wave equation (1) be discretized in space and in time by a pair of Gauss-Legendre collocation methods with s, r respectively, stages. Then the resulting discretization is a multi-symplectic integrator with discrete conservation law (29).

It might appear as if the order in which the discretization in space and time is carried out would lead to different schemes. But this is not the case. Take, for example, the spatial discretization (16)-(19), which we write in its time-sampled version

$$U_{i,m} = u_0^m + \Delta x \sum_{j=1}^{s} a_{ij} W_{j,m}, \tag{31}$$

$$W_{i,m} = w_0^m + \Delta x \sum_{j=1}^{s} a_{ij} \left(\partial_t V_{j,m} + V'(U_{j,m})\right), \tag{32}$$

$$u_1^m = u_0^m + \Delta x \sum_{i=1}^{s} b_i W_{i,m}, \tag{33}$$

$$w_1^m = w_0 + \Delta x \sum_{i=1}^{s} b_i \left(\partial_t V_{i,m} + V'(U_{i,m})\right), \tag{34}$$

and the time discretization (25)-(28). We could apply the substitution

$$\partial_x W_{i,m} = \partial_t V_{i,m} + V'(U_{i,m})$$

in (32) and (34) as well as

$$\partial_t V_{i,m} = \partial_x W_{i,m} - V'(U_{i,m})$$

in (26) and (28) to obtain the same scheme which, however, appears now to be obtained via a semi-discretization in time followed by a discretization in space. In fact, our schemes can be written in the general form as presented in Fig. 1.

We like to point out that $s = r = 1$, i.e., an implicit midpoint discretization in space and time, leads to the centered Preissmann scheme[1] [1, 6]

$$\frac{1}{\Delta t}\mathbf{M}\left(\boldsymbol{z}_{1/2}^{1} - \boldsymbol{z}_{1/2}^{0}\right) + \frac{1}{\Delta x}\mathbf{K}\left(\boldsymbol{z}_{1}^{1/2} - \boldsymbol{z}_{0}^{1/2}\right) = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}_{1/2}^{1/2}) \tag{35}$$

when applied to a general multi-symplectic PDE (2). Here the standard abbreviations

$$\boldsymbol{z}_{1/2}^{0} = \frac{1}{2}\left(\boldsymbol{z}_0^0 + \boldsymbol{z}_1^0\right), \quad \boldsymbol{z}_0^{1/2} = \frac{1}{2}\left(\boldsymbol{z}_0^0 + \boldsymbol{z}_0^1\right), \quad \boldsymbol{z}_{1/2}^{1/2} = \frac{1}{4}\left(\boldsymbol{z}_1^1 + \boldsymbol{z}_1^0 + \boldsymbol{z}_0^1 + \boldsymbol{z}_0^0\right) \quad \text{etc.}$$

are used. The corresponding discrete multi-symplectic conservation law is [6]

$$\left[\boldsymbol{dz}_{1/2}^{1} \wedge \mathbf{M}\boldsymbol{dz}_{1/2}^{1} - \boldsymbol{dz}_{1/2}^{0} \wedge \mathbf{M}\boldsymbol{dz}_{1/2}^{0}\right]\Delta x + \left[\boldsymbol{dz}_{1}^{1/2} \wedge \mathbf{K}\boldsymbol{dz}_{1}^{1/2} - \boldsymbol{dz}_{0}^{1/2} \wedge \mathbf{K}\boldsymbol{dz}_{0}^{1/2}\right]\Delta t = 0.$$

See [6] for a detailed discussion of the Preissmann scheme and its application to multi-symplectic PDEs (2).

When looking at problems with periodic boundary conditions, formula (29) has another interesting consequence. Let us take the sum of the equation (29) over all spatial grid points $k = 1, \ldots, M$

$$\sum_{k=1}^{M}\left(\sum_{i=1}^{s} b_i \left[\boldsymbol{du}_{i,k}^{1} \wedge \boldsymbol{dv}_{i,k}^{1} - \boldsymbol{du}_{i,k}^{0} \wedge \boldsymbol{dv}_{i,k}^{0}\right]\Delta x - \sum_{m=1}^{r} \tilde{b}_m \left[\boldsymbol{du}_{k+1}^{m} \wedge \boldsymbol{dw}_{k+1}^{m} - \boldsymbol{du}_{k}^{m} \wedge \boldsymbol{dw}_{k}^{m}\right]\Delta t\right) = 0.$$

[1] Preissmann originally suggested the method in 1961 for the solution of one dimensional open-channel hydraulics problems. The scheme is a popular choice for the computation of unsteady flow problems. It is less well-known that the scheme can also be applied to wave equations (see [1] for a historical account).

$$
\begin{aligned}
U_{i,m} &= u_0^m + \Delta x \sum_{j=1}^{s} a_{ij} \partial_x U_{j,m}, \\
W_{i,m} &= w_0^m + \Delta x \sum_{j=1}^{s} a_{ij} \partial_x W_{j,m}, \\
u_1^m &= u_0^m + \Delta x \sum_{i=1}^{s} b_i \partial_x U_{i,m}, \\
w_1^m &= w_0 + \Delta x \sum_{i=1}^{s} b_i \partial_x W_{i,m},
\end{aligned}
$$

$$
\begin{aligned}
U_{i,m} &= u_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t U_{i,n}, \\
V_{i,m} &= v_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t V_{i,n}, \\
u_i^1 &= u_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t U_{i,m}, \\
v_i^1 &= v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t V_{i,m},
\end{aligned}
$$

$$
\begin{aligned}
\partial_t U_{i,m} &= V_{i,m}, \\
\partial_x U_{i,m} &= W_{i,m}, \\
\partial_t V_{i,m} - \partial_x W_{i,m} &= -V'(U_{i,m}).
\end{aligned}
$$

Figure 1: Multi-Symplectic Gauss-Legendre Collocation Methods for Nonlinear Wave Equation.

Here we have used the abbreviations

$$u_{i,k}^1 \approx u(c_i \Delta x + k\Delta x, \Delta t), \qquad u_k^m \approx u(k\Delta x, d_m \Delta t)$$

etc. Periodicity in space implies

$$\sum_{k=1}^{M} \sum_{m=1}^{r} \tilde{b}_m \left[\boldsymbol{d}u_{k+1}^m \wedge \boldsymbol{d}w_{k+1}^m - \boldsymbol{d}u_k^m \wedge \boldsymbol{d}w_k^m \right] \Delta t = \sum_{m=1}^{r} \tilde{b}_m \left[\boldsymbol{d}u_{M+1}^m \wedge \boldsymbol{d}w_{M+1}^m - \boldsymbol{d}u_1^m \wedge \boldsymbol{d}w_1^m \right] \Delta t = 0$$

which in turn yields

$$\sum_{k=1}^{M} \sum_{i=1}^{s} b_i \boldsymbol{d}u_{i,k}^1 \wedge \boldsymbol{d}v_{i,k}^1 = \sum_{k=1}^{M} \sum_{i=1}^{s} b_i \boldsymbol{d}u_{i,k}^0 \wedge \boldsymbol{d}v_{i,k}^0.$$

This is precisely conservation of symplecticity in time with respect to the state variables

$$\boldsymbol{u} = \{u_{i,k}\}_{k=1,\ldots M; i=1,\ldots,s} \quad \text{and} \quad \boldsymbol{v} = \{v_{i,k}\}_{k=1,\ldots M; i=1,\ldots,s}$$

and the wedge product $\boldsymbol{du} \wedge \boldsymbol{Bdv}$ where $\boldsymbol{B}$ is a diagonal matrix with entries corresponding to the weights $\{b_i\}$. In other words, multi-symplectic Gauss-Legendre methods imply the conservation of symplecticity in time, i.e.

$$\boldsymbol{du}^{n+1} \wedge \boldsymbol{Bdv}^{n+1} = \boldsymbol{du}^n \wedge \boldsymbol{Bdv}^n,$$

when applied to problems with periodic boundary conditions. Thus these methods are also symplectic discretizations in the "classical" sense (although with a non-canonical - but non-degenerate - symplectic structure).

Proposition 2. Let the multi-symplectic formulation (10)-(12) of the nonlinear wave equation (1) be discretized in space and in time by a pair of Gauss-Legendre collocation methods with s, r respectively, stages. Assume that we solve an initial value problem in time with periodic boundary conditions in space. Then the resulting discretization yields a finite dimensional Hamiltonian truncation of the wave equation in space with the underlying symplectic structure $\boldsymbol{du} \wedge \boldsymbol{Bdv}$ and a symplectic discretization of this finite-dimensional system in time.

3 Conservation of Energy and Momentum

As already mentioned in the Introduction, the wave equation (1) satisfies the energy conservation law

$$\partial_t E + \partial_x F = 0$$

where

$$E = \frac{1}{2}\left(w^2 + v^2\right) + V(u)$$

is the energy density and

$$F = -vw$$

is the energy flux. The wave equation also satisfies the momentum conservation law (9). We will come back to the issue of momentum conservation towards the end of this section.

We now check for the conservation of the following discrete energy conservation law

$$\sum_{i=1}^{s} b_i \left[E_i^1 - E_i^0\right] \Delta x + \sum_{m=1}^{r} \tilde{b}_m \left[F_1^m - F_0^m\right] \Delta t = 0 \tag{36}$$

with the obvious abbreviations

$$E_i^1 = \frac{1}{2}\left(\left(w_i^1\right)^2 + \left(v_i^1\right)^2\right) + V(u_i^1), \qquad F_1^m = -v_1^m w_1^m,$$

etc. This is an approximation to the contour integral in the (x,t) plane

$$\int_{x=0}^{k\Delta x} \left[E(\boldsymbol{z}(x, n\Delta t)) - E(\boldsymbol{z}(x,0))\right] dx + \int_{t=0}^{n\Delta t} \left[F(\boldsymbol{z}(k\Delta x, t)) - F(\boldsymbol{z}(0,t))\right] dt = 0 \tag{37}$$

with $k = n = 1$ in the same sense as (29) is for (30). It immediately also implies a corresponding result for any $k, n > 1$.

Since Gauss-Legendre collocation methods preserve quadratic integrals of ODEs exactly [7, 18], we could expect that multi-symplectic Gauss-Legendre methods will give rise to a discrete conservation law (36) when $V(u) = cu^2/2$, $c \in \mathbb{R}$ some constant. To be able to evaluate the corresponding discrete conservation law (36), we have to first introduce two auxiliary systems, namely

$$V_{i,m} = v_0^m + \Delta x \sum_{j=1}^{s} a_{ij} \partial_x V_{j,m}, \tag{38}$$

$$v_1^m = v_0^m + \Delta x \sum_{i=1}^{s} b_i \partial_x V_{i,m} \tag{39}$$

and

$$W_{i,m} = w_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t W_{i,n}, \tag{40}$$

$$w_i^1 = w_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t W_{i,m} \tag{41}$$

to obtain the missing approximations of v and w along the boundary of $[0, \Delta x] \times [0, \Delta t]$. The undetermined values of $\{v_0^m\}$ and $\{w_i^0\}$ are implicitly given by

$$u_0^m = u_0^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} v_0^n \tag{42}$$

and

$$u_i^0 = u_0^0 + \Delta x \sum_{j=1}^{s} a_{ij} w_j^0. \tag{43}$$

Using the equations (38)-(41), (25), and (31), we derive the two identities

$$\begin{aligned}
U_{i,m} &= u_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} V_{i,n} \\
&= u_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \left(v_0^n + \Delta x \sum_{j=1}^{s} a_{ij} \partial_x V_{j,n} \right) \\
&= u_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} v_0^n + \Delta t \Delta x \sum_{j=1}^{s} \sum_{n=1}^{r} a_{ij} \tilde{a}_{mn} \partial_x V_{j,n} \\
&= u_i^0 + u_0^m - u_0^0 + \Delta t \Delta x \sum_{j=1}^{s} \sum_{n=1}^{r} a_{ij} \tilde{a}_{mn} \partial_x V_{j,n}
\end{aligned}$$

and, similarly,

$$U_{i,m} = u_0^m + u_i^0 - u_0^0 + \Delta t \Delta x \sum_{j=1}^{s} \sum_{n=1}^{r} a_{ij} \tilde{a}_{mn} \partial_t W_{j,n}.$$

This implies

$$\sum_{j=1}^{s} \sum_{n=1}^{r} a_{ij} \tilde{a}_{mn} \partial_x V_{j,n} = \sum_{j=1}^{s} \sum_{n=1}^{r} a_{ij} \tilde{a}_{mn} \partial_t W_{j,n}$$

and we can conclude that

$$\partial_x V_{i,m} = \partial_t W_{i,m} \qquad \text{for all } i, m. \tag{44}$$

This reflects the fact that the exact solutions also satisfy $\partial_x v = \partial_t w = \partial_{xt} u$. (In [6], this "hidden" conservation law is made explicit by going to a different multi-symplectic formulation of the wave equation (1).)

Note that we also obtain the additional equations

$$u_0^1 = u_0^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m v_0^m \quad \text{and} \quad u_1^0 = u_0^0 + \Delta x \sum_{i=1}^{s} b_i w_i^0$$

as well as

$$u_1^1 = u_1^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m v_1^m \quad \text{and} \quad u_1^1 = u_0^1 + \Delta x \sum_{i=1}^{s} b_i w_i^1.$$

which define $u_0^0 \approx u(0,0)$, $u_1^0 \approx u(\Delta x, 0)$, $u_0^1 \approx u(0, \Delta t)$, and $u_1^1 \approx u(\Delta x, \Delta t)$ and thus close the auxiliary system (38)-(43). These equations are over-determined but self-consistent because of

$$\begin{aligned} 0 &= \Delta t \sum_{m=1}^{r} \tilde{b}_m v_1^m + \Delta x \sum_{i=1}^{s} b_i w_i^0 - \Delta t \sum_{m=1}^{r} \tilde{b}_m v_0^m - \Delta x \sum_{i=1}^{s} b_i w_i^1 \\ &= \Delta t \sum_{m=1}^{r} \tilde{b}_m v_0^m + \Delta t \Delta x \sum_{m=1}^{r} \sum_{i=1}^{s} \tilde{b}_m b_i \partial_x V_{i,m} + \Delta x \sum_{i=1}^{s} b_i w_i^0 - \\ &\quad - \Delta t \sum_{m=1}^{r} \tilde{b}_m v_0^m - \Delta x \sum_{i=1}^{s} b_i w_i^0 - \Delta x \Delta t \sum_{i=1}^{s} \sum_{m=1}^{r} b_i \tilde{b}_m \partial_t W_{i,m} \end{aligned}$$

and (44). In fact, we have just shown that the "hidden" conservation law $v_t - w_x = 0$ gives rise to the discrete conservation law

$$\sum_{m=1}^{r} \tilde{b}_m \left[v_1^m - v_0^m \right] \Delta t - \sum_{i=1}^{s} b_i \left[w_i^1 - w_i^0 \right] \Delta x = 0.$$

Let us now come back to the discrete energy conservation law (36). The equations (38)-(41) together with (31)-(34) and (25)-(28) yield

$$\begin{aligned} w_1^m v_1^m &= \left(w_0^m + \Delta x \sum_{i=1}^{s} b_i \left(\partial_t V_{i,m} + c U_{i,m} \right) \right) \left(v_0^m + \Delta x \sum_{i=1}^{s} b_i \partial_x V_{i,m} \right) \\ &= w_0^m v_0^m + \Delta x \sum_{i=1}^{s} b_i \left(V_{i,m} \partial_t V_{i,m} + c V_{i,m} U_{i,m} + W_{i,m} \partial_x V_{i,m} \right) \end{aligned} \tag{45}$$

and, similarly,

$$E_i^1 = E_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \left(V_{i,m} \partial_t V_{i,m} + c U_{i,m} V_{i,m} + W_{i,m} \partial_t W_{i,m} \right) \tag{46}$$

where we used the fact that

$$b_j a_{ji} + b_i a_{ij} - b_i b_j = 0 \quad \text{and} \quad \tilde{b}_j \tilde{a}_{ji} + \tilde{b}_i \tilde{a}_{ij} - \tilde{b}_i \tilde{b}_j = 0$$

in the same manner as done in §2 to prove multi-symplecticity. Combining both formulas, we obtain

$$\sum_{i=1}^{s} b_i \left[E_i^1 - E_i^0 \right] \Delta x + \sum_{m=1}^{r} \tilde{b}_m \left[F_1^m - F_0^m \right] \Delta t = \sum_{i=1}^{s} \sum_{m=1}^{r} b_i \tilde{b}_m W_{i,m} \left(\partial_t W_{i,m} - \partial_x V_{i,m} \right).$$

The right hand side of this equation is zero due to (44).

Proposition 3. Let the multi-symplectic formulation (10)-(12) of the nonlinear wave equation (1) be discretized in space and in time by a pair of Gauss-Legendre collocation methods with s, r respectively, stages. Let us also assume that the potential V in (1) is of the form

$$V(u) = \frac{c}{2}u^2,$$

$c \in \mathbb{R}$ some constant. Then the resulting discretization conserves the discrete energy conservation law (36).

Li & Vu-Quoc have suggested a method that exactly conserves a discrete local energy conservation law for any type of smooth potential $V(u)$ [21, 15]. This local energy conservation law is, however, different from (36). Their approach is based on a second central difference approximation in space and an energy conserving variant of the implicit midpoint method in time. We wish to point out that, following their approach, one can also obtain a variant of the centered Preissmann scheme (35) that exactly conserves the discrete energy conservation law (36) with $s = r = 1$ for any smooth potential $V(u)$. The idea is to apply an implicit midpoint discretization in space and a proper energy conserving variant of the midpoint discretization in time. See the Appendix for more details. Note that this energy conserving scheme cannot be expected to be multi-symplectic, in general, and that, for linear problems, the scheme reduces to the box scheme.

We now investigate the preservation of the momentum conservation law (9). We first define a discrete conservation law

$$\sum_{i=1}^{s} b_i \left[I_i^1 - I_i^0\right] \Delta x + \sum_{m=1}^{r} \tilde{b}_m \left[G_1^m - G_0^m\right] \Delta t = 0 \tag{47}$$

with the obvious abbreviations

$$I_i^1 = -w_i^1 v_i^1, \qquad G_1^m = \frac{1}{2}\left((v_1^m)^2 + (w_1^m)^2\right) - V(u_1^m),$$

etc. This is an approximation to the contour integral in the (x,t) plane,

$$\int_{x=0}^{\Delta x} [I(z(x,\Delta t)) - I(z(x,0))]\, dx + \int_{t=0}^{\Delta t} [G(z(\Delta x,t)) - G(z(0,t))]\, dt = 0.$$

Assuming $V(u) = cu^2/2$, we first derive

$$\begin{aligned} w_i^1 v_i^1 &= \left(w_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t W_{i,m}\right)\left(v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t V_{i,m}\right) \\ &= w_i^0 v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \left(V_{i,m}\partial_x V_{i,m} + W_{i,m}\partial_t V_{i,m}\right) \\ &= w_i^0 v_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \left(V_{i,m}\partial_x V_{i,m} + W_{i,m}\partial_x W_{i,m} - cW_{i,m}U_{i,m}\right) \end{aligned}$$

where, in the second line, we made use of (44). We also obtain

$$G_1^m = G_0^m + \Delta x \sum_{i=1}^{s} b_i \left(W_{i,m}\partial_x W_{i,m} + V_{i,m}\partial_x V_{i,m} - cU_{i,m}W_{i,m}\right)$$

Combining both results, we indeed obtain the discrete conservation law (47).

Proposition 4. Let the multi-symplectic formulation (10)-(12) of the nonlinear wave equation (1) be discretized in space and in time by a pair of Gauss-Legendre collocation methods with s, r respectively, stages. Let us also assume that the potential V in (1) is of the form

$$V(u) = \frac{c}{2}u^2,$$

$c \in \mathbb{R}$ some constant. Then the resulting discretization conserves the discrete momentum conservation law (47).

Proposition 3 & 4 show that multi-symplectic integrators for linear wave equations have excellent energy-momentum conservation. This suggests that multi-symplectic integrators for nonlinear wave equations will preserve the discrete energy-momentum conservation laws in good approximation.

The following "global" result for a wave equation (1) with periodic boundary conditions $u(0,t) = u(L,t)$ can be stated. It follows from (37) that

$$\mathcal{E}(t) := \int_{x=0}^{L} E(\boldsymbol{z}(x,t))dx = \mathcal{E}(0) := \int_{x=0}^{L} E(\boldsymbol{z}(x,0))dx$$

if $\boldsymbol{z}(0,t) = \boldsymbol{z}(L,t)$ (periodic boundary conditions). This implies conservation of total energy $\mathcal{E}(t)$ for the wave equation when considered as an infinite-dimensional Hamiltonian PDE. Any finite-dimensional Hamiltonian approximation of the wave equation and subsequent symplectic integration in time will conserve this energy very well provided Δt small enough [2]. This also applies to the multi-symplectic Gauss-Legendre methods of §2 which follows from Proposition 2 and backward error analysis results in [2, 16]. Furthermore, there is also conservation of global momentum

$$\mathcal{I}(t) := \int_{x=0}^{L} I(\boldsymbol{z}(x,t))dx = \mathcal{I}(0) := \int_{x=0}^{L} I(\boldsymbol{z}(x,0))dx$$

if $\boldsymbol{z}(0,t) = \boldsymbol{z}(L,t)$ (periodic boundary conditions). Since $\mathcal{I}$ is a quadratic expression in v and w, Gauss-Legendre collocation methods will preserve the discrete global momentum conservation law exactly.

However, this global view provides a much weaker concept of energy and momentum conservation. It is a necessary but not sufficient condition for the preservation of the corresponding local conservation laws.

4 Semi-Explicit and Linearly Implicit Multi-Symplectic Discretizations

There are certainly other options available for the time discretization then using a high-order implicit Gauss-Legendre collocation method (25)-(28) when integrating an initial-boundary value (Cauchy) problem. In fact, one can either apply the implicit midpoint method in time and use appropriate concatenations of the corresponding scheme to obtain a higher order in time method or one can apply a higher order explicit symplectic partitioned Runge-Kutta method in time [18]. Let us, for example, take an explicit symplectic concatenation method of the form

$$\begin{aligned} & U_{i,1} = u_i^0, \\ & V_{i,1} = v_i^0, \\ \text{for } m = 1,\ldots,r \qquad & U_{i,m+1} = U_{i,m} + \alpha_m \Delta t V_{i,m+1}, \\ & V_{i,m+1} = V_{i,m} + \beta_m \Delta t \partial_t V_{i,m}, \\ & u_i^1 = U_{i,r+1}, \\ & u_i^1 = V_{i,r+1} \end{aligned}$$

with weights (α_m, β_m). This yields

$$\left[\boldsymbol{d}u_i^1 \wedge \boldsymbol{d}v_i^1 - \boldsymbol{d}u_i^0 \wedge \boldsymbol{d}v_i^0\right] - \sum_{m=1}^{r} \beta_m \left[\boldsymbol{d}U_{i,m} \wedge \partial_t \boldsymbol{d}V_{i,m}\right] \Delta t = 0$$

which in turn implies the discrete conservation law

$$\sum_{i=1}^{s} b_i \left[\boldsymbol{d}u_i^1 \wedge \boldsymbol{d}v_i^1 - \boldsymbol{d}u_i^0 \wedge \boldsymbol{d}v_i^0\right] \Delta x - \sum_{m=1}^{r} \beta_m \left[\boldsymbol{d}u_1^m \wedge \boldsymbol{d}w_1^m - \boldsymbol{d}u_0^m \wedge \boldsymbol{d}w_0^m\right] \Delta t = 0$$

which is again a discretization of (30).

Another option is to apply the multi-symplectic Gauss-Legendre collocation methods from Fig. 1 to a linearized wave equation and to use the following three step discretization for the nonlinear problem:

1. Update v_i^0 via
$$\tilde{v}_i^0 = v_i^0 - \frac{\Delta t}{2} \bar{V}'(u_i^0)\,.$$
2. Apply a multi-symplectic Gauss-Legendre method to the linearized wave equation using $\tilde{v}_i^0$. Denote the result by $(u_1^m, w_1^m, u_i^1, \tilde{v}_i^1)^T$.
3. Update $\tilde{v}_i^1$ via
$$v_i^1 = \tilde{v}_i^1 - \frac{\Delta t}{2} \bar{V}'(u_i^1)\,.$$

Here $V(u) = cu^2/2 + \bar{V}(u)$ was used. This linearly implicit scheme conserves the multi-symplectic conservation law (29). The overall scheme will only be second order in time, in general. But higher order in time schemes can be obtained by a proper composition of the (symmetric) second order scheme [14].

5 Numerical Experiments

To gain insight into the performance of the suggested multi-symplectic methods, in particular into their local conservation of energy and momentum, we perform the following numerical experiments. We discretize the sine-Gordon equation

$$\partial_{tt} u = \partial_{xx} u - \sin(u)$$

using the multi-symplectic Gauss-Legendre method with $r = 1$ (midpoint in time) and $s = 2$ (fourth order Gauss-Legendre method in space). We implement periodic boundary conditions $u(-L/2, t) = u(L/2, t)$ for two different sets of initial conditions. For the first experiment, which we call *Experiment A*, we use $L = 100$,

$$u(x,0) = 4\tan^{-1}\left(\frac{e^{x-L/6}}{\sqrt{1-\beta^2}}\right) + 4\tan^{-1}\left(\frac{e^{-x-L/6}}{\sqrt{1-\beta^2}}\right),$$

and

$$v(x,0) = \frac{\partial}{\partial t}\left[4\tan^{-1}\left(\frac{e^{x-L/6-\beta t}}{\sqrt{1-\beta^2}}\right) + 4\tan^{-1}\left(\frac{e^{-x-L/6-\beta t}}{\sqrt{1-\beta^2}}\right)\right]_{t=0}.$$

On an infinite domain, these initial conditions correspond to a soliton and anti-soliton solution moving with speed $\pm\beta$. We set $\beta = 0.5$. In Fig. 2, snapshots of the time evolution of the wave form

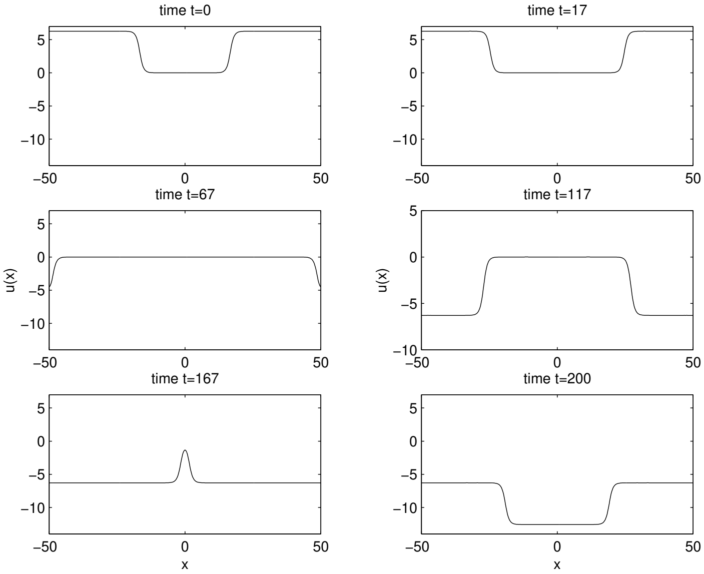

Figure 2: Time evolution of the soliton/anti-soliton solution over the time interval $t \in [0, 200]$.

$u(x,t)$ are shown over a time interval $t \in [0, 200]$. This approximation is obtained using a time-step of $\Delta t = 0.1$ and $M = 100$ spatial mesh points.

For the second experiment, called *Experiment B*, we consider the so-called breather solution

$$u(x,t) = 4\tan^{-1}\left(\frac{\sqrt{1-\omega^2}}{\omega}\frac{\cos \omega t}{\cosh\left(x\sqrt{1-\omega^2}\right)}\right)$$

with $\omega = 0.9$. On an infinite domain, this is a bump shaped solution which oscillates up and down with period $2\pi/\omega$. To exclude boundary effects, we used period boundary conditions with $L = 100$.

We monitor the drift in the numerical approximations to the total energy $\mathcal{E}(t)$ and the total momentum $\mathcal{I}(t)$ as well as the error in the numerical discretizations of the local energy conservation law (36) and the local momentum conservation law (47).

The numerical errors in the conserved quantities for the Experiment A can be found in Fig. 3. These results are obtained using $M = 100$ spatial grid points and a time-step of $\Delta t = 0.1$. Total momentum $\mathcal{I}(t)$ is conserved exactly since it is a quadratic invariant. The two pronounced spikes in the error of the total energy correspond to rapid "flip" transitions of the solution $u(x,t)$ whenever the two kinks meet at $x = \pm L$ or $x = 0$.

We also plot the error in the local conservation laws (36) and (47) as a function of the spatial grid location and the time step. As can be seen from Fig. 4, the errors are mainly concentrated around the two moving fronts.

The corresponding numerical results for the Experiment B can be found in Fig. 5. These results are obtained using $M = 60$ spatial grid points and 60 time steps per period of the motion which is $T = 2\pi/\omega \approx 6.9813$. Again, total momentum $\mathcal{I}(t)$ is conserved exactly (up to the error in the Newton iteration) since it is a quadratic invariant. The error behaviour of the total energy is typical for a symplectic time discretization of an Hamiltonian ODE. The errors in the local conservation laws are focused about $x = 0$ where the center of the breather solution is located. Instead of summing the errors in the local conservation laws over the full spatial extension and plotting the result as a function of time, one can also sum the errors over a fixed spatial interval $[0, a]$ and time intervals $[0, \tau]$, $\tau \geq 0$. See Fig. 6 for the case $\tau \in [0, 140]$ and $a = L/4$. Note that the errors in the local

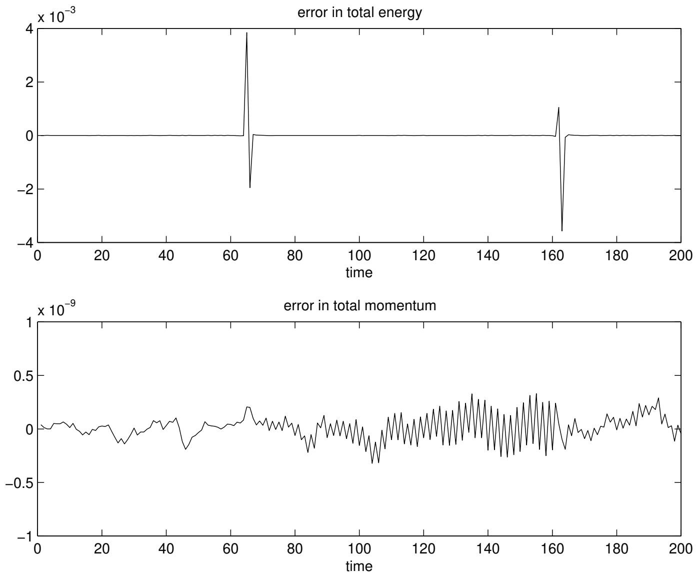

Figure 3: Numerical errors in the global energy and momentum over the time interval $[0, 200]$ (with two collisions of kinks).

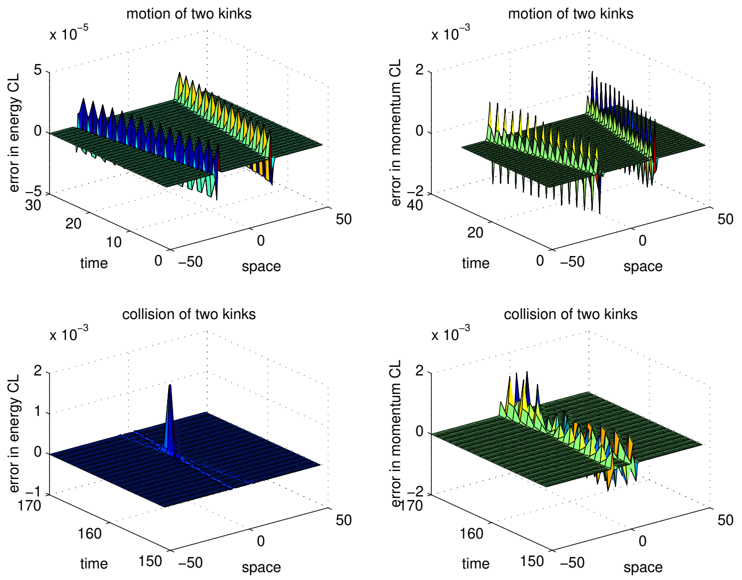

Figure 4: Numerical errors in the local energy/momentum conservation laws over the two intervals $[0, 30]$ (no collision of kinks) and $[150, 170]$ (collision of kinks at $x = 0$).

energy conservation law do not grow with τ but that the corresponding errors in the momentum conservation laws increase with increasing values of τ.

We like to point out that our numerical experiments show that the error in the energy conservation law (36) divided by the area element $\Delta x \Delta t$ depends only on the chosen time-step Δt and is second order in Δt while the corresponding error in the local momentum conservation law (47) depends only on the spatial mesh-size Δx and is approximately of fourth order in Δx. See Table 5.

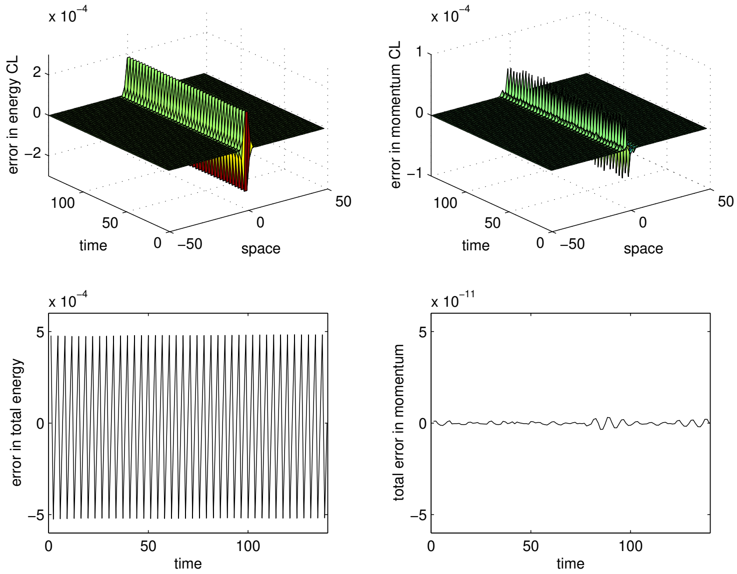

Figure 5: Numerical errors in the local/global energy/momentum conservation laws for the breather solution over the time interval $[0, 140]$.

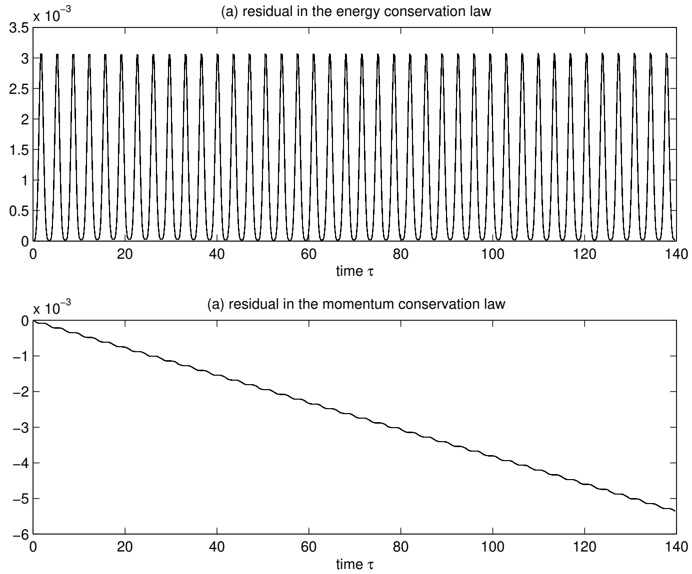

Figure 6: Numerical errors in the local energy (a) and momentum (b) conservation laws summed over the spatial interval $[0, L/4]$ and time intervals $[0, \tau]$ as a function of $\tau \in [0, 140]$ (breather solution).

For comparison, we implemented a method-of-line approach to the wave equation (1) using the Störmer-Verlet method [18] in time and the symmetric fourth order finite differences discretization of the Laplacian operator [8]. The resulting discretization can be written as

$$q_j^{n+1} = q_j^n + \Delta t p_j^{n+1/2} ,$$

Energy/Momentum	$\Delta t = 0.058$	$\Delta t = 0.116$	$\Delta t = 0.1745$
$\Delta x = 1.0$	3.2e-4/4.16e-5	1.3e-3 4.09e-5	2.8e-3/4.06e-5
$\Delta x = 1.25$	3.03e-4/1.06e-4	1.2e-3/1.06e-4	2.7e-3/1.04e-4
$\Delta x = 1.67$	3.06e-4/2.72e-4	1.1e-3/2.97e-4	2.4e-3/2.87e-4

Figure 7: Maximum error in the local energy/momentum conservation laws over all spatial grid points and two time periods as a function of the spatial mesh size Δx and the time step Δt. The residuals in (36) and (47) are divided by $\Delta t \Delta x$ to make the corresponding integrals independent of the size of the cell over which they are taken.

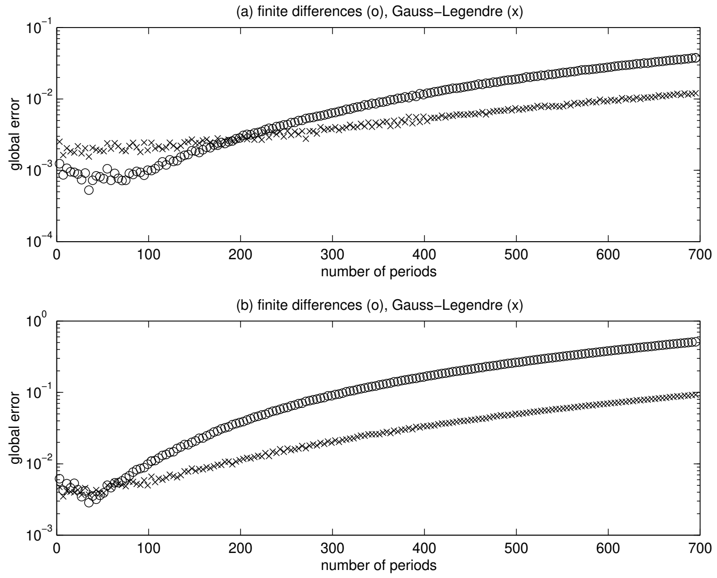

Figure 8: Global solution error for the breather solution after $k = 1, \ldots, 700$ periods for $\Delta t = T/120$ and different values of $\Delta x = L/M$ using a symplectic finite differences method and a multi-symplectic Gauss-Legendre collocation method of the same order: (a) Gauss-Legendre method (x) with $M = 100$ and finite differences method (o) with $M = 150$ mesh points; (b) Gauss-Legendre method (x) with $M = 80$ and finite differences method (o) with $M = 100$ mesh points.

$$p_j^{n+1/2} \quad = \quad p_j^{n-1/2} + \frac{\Delta t}{\Delta x^2}\left(\frac{-q_{j+2}^n + 16q_{j+1}^n - 30q_j^n + 16q_{j-1}^n - q_{j-2}^n}{12}\right) - \Delta t V'(q_j^n)\,.$$

As shown in [13, 8], the resulting method is symplectic when considered as a time discretization of a finite dimensional Hamiltonian approximation of (1). However, because of the non-symplectic finite difference approximation of the Laplacian, the overall method is not multi-symplectic. We repeated the Experiment B with this finite differences scheme and evaluated the l_∞ global error of the numerical computed breather solution after k periods, $k = 1, \ldots, 700$. The results for a step-size of $\Delta t = T/120$, $T = 2\pi/\omega$, and different values of the spatial mesh-size $\Delta x = L/M$, $L = 100$, can be found in Fig. 8. We note that the symplectic finite differences method has initially a smaller global error compared to the multi-symplectic Gauss-Legendre collocation method. However, due to an apparently more favourable error propagation, the multi-symplectic collocation method yields, in both cases, a smaller global error after $k = 700$ periods. Note that both methods use a second order discretization in time and a fourth order discretization in space.

6 Another Example: Nonlinear Schrödinger Equation

To demonstrate the generality of our approach, we briefly consider multi-symplectic integration of the one dimensional nonlinear Schrödinger equation [5]

$$\mathrm{i}\partial_t \psi = \partial_{xx}\psi + V'(|\psi|^2)\psi, \qquad (x,t) \in \mathcal{U} \subset \mathbb{R}^2,$$

$V : \mathbb{R} \to \mathbb{R}$ some smooth function. Using $\psi = a + ib$, we rewrite this as a pair of real-valued equations

$$\begin{aligned} \partial_t a &= +\partial_{xx} b + V'(a^2+b^2)b, \\ \partial_t b &= -\partial_{xx} a - V'(a^2+b^2)a. \end{aligned}$$

Next we introduce a pair of conjugate momenta $v = a_x$, $w = b_x$, and obtain the multi-symplectic PDE

$$\begin{aligned} -\partial_t b - \partial_x v &= V'(a^2+b^2)a, \\ \partial_t a - \partial_x w &= V'(a^2+b^2)b, \\ \partial_x a &= v, \\ \partial_x b &= w \end{aligned}$$

with phase space variable $\boldsymbol{z} = (a,b,v,w)^T$ and Hamiltonian

$$S(\boldsymbol{z}) = \frac{1}{2}\left(v^2 + w^2 + V(a^2+b^2)\right).$$

The corresponding multi-symplectic conservation law (3) is

$$\partial_t \left[\boldsymbol{d}a \wedge \boldsymbol{d}b\right] + \partial_x \left[\boldsymbol{d}a \wedge \boldsymbol{d}v + \boldsymbol{d}b \wedge \boldsymbol{d}w\right] = 0. \tag{48}$$

We like to point out that one of the conservation laws of the Schrödinger equation is

$$\partial_t \frac{a^2+b^2}{2} + \partial_x (vb - wa) = 0\,. \tag{49}$$

Again we first discretize the reformulated equation

$$\begin{aligned} \partial_x v &= -\partial_t b - V'(a^2+b^2)a, \\ \partial_x w &= +\partial_t a - V'(a^2+b^2)b, \\ \partial_x a &= v, \\ \partial_x b &= w \end{aligned}$$

in space by a Gauss-Legendre collocation method. Using similar notations as in §2, it is relatively straightforward to derive the corresponding semi-discretized conservation law

$$[\boldsymbol{d}a_1 \wedge \boldsymbol{d}v_1 - \boldsymbol{d}a_0 \wedge \boldsymbol{d}v_0] + [\boldsymbol{d}b_1 \wedge \boldsymbol{d}w_1 - \boldsymbol{d}b_0 \wedge \boldsymbol{d}w_0] + \sum_{i=1}^{s} b_i \partial_t \left[\boldsymbol{d}A_i \wedge \boldsymbol{d}B_i\right] \Delta x = 0.$$

Discretization in time is now achieved by using

$$\begin{aligned} A_{i,m} &= a_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t A_{i,n}, \\ B_{i,m} &= b_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t B_{i,n}, \\ a_i^1 &= a_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t A_{i,m}, \\ b_i^1 &= b_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t B_{i,m} \end{aligned}$$

with corresponding conservation property

$$\left[\boldsymbol{d}a_i^1 \wedge \boldsymbol{d}b_i^1 - \boldsymbol{d}a_i^0 \wedge \boldsymbol{d}b_i^0\right] - \sum_{m=1}^{r} \tilde{b}_m \left[\partial_t \boldsymbol{d}A_{i,m} \wedge \boldsymbol{d}B_{i,m} + \boldsymbol{d}A_{i,m} \wedge \partial_t \boldsymbol{d}B_{i,m}\right] \Delta t = 0.$$

Combining these results, we derive the discretized multi-symplectic conservation law

$$\begin{aligned} &\sum_{i=1}^{s} b_i \left[\boldsymbol{d}a_i^1 \wedge \boldsymbol{d}b_i^1 - \boldsymbol{d}a_i^0 \wedge \boldsymbol{d}b_i^0\right] \Delta x + \\ &\quad + \sum_{r=1}^{m} \tilde{b}_m \left[\boldsymbol{d}a_1^m \wedge \boldsymbol{d}v_1^m - \boldsymbol{d}a_0^m \wedge \boldsymbol{d}v_0^m + \boldsymbol{d}b_1^m \wedge \boldsymbol{d}w_1^m - \boldsymbol{d}b_0^m \wedge \boldsymbol{d}w_0^m\right] \Delta t \quad = \quad 0 \end{aligned}$$

which is a discretization of (48) integrated over the domain $[0, \Delta x] \times [0, \Delta t]$.

Using the complex-valued state variable $\boldsymbol{z} = (\psi, \phi)^T \in \mathbb{C}^2$, $\partial_x \psi = \phi$, we can rewrite the multi-symplectic formulation of the nonlinear Schrödinger equation in a more compact notation as

$$\begin{aligned} \mathrm{i}\partial_t \psi - \partial_x \phi &= V'(|\psi|^2)\psi, \\ \partial_x \psi &= \phi \end{aligned}$$

and the general form of a multi-symplectic Gauss-Legendre discretization can be found in Fig. 9.

$$\begin{aligned} \Psi_{i,m} &= \psi_0^m + \Delta x \sum_{j=1}^{s} a_{ij} \partial_x \Psi_{j,m}, \\ \Phi_{i,m} &= \phi_0^m + \Delta x \sum_{j=1}^{s} a_{ij} \partial_x \Phi_{j,m}, \\ \psi_1^m &= \psi_0^m + \Delta x \sum_{i=1}^{s} b_i \partial_x \Psi_{i,m}, \\ \phi_1^m &= \phi_0 + \Delta x \sum_{i=1}^{s} b_i \partial_x \Phi_{i,m}, \end{aligned}$$

$$\begin{aligned} \Psi_{i,m} &= \psi_i^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t \Psi_{i,n}, \\ \psi_i^1 &= \psi_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t \Psi_{i,m}, \end{aligned}$$

$$\begin{aligned} \mathrm{i}\partial_t \Psi_{i,m} - \partial_x \Phi_{i,m} &= V'(|\Psi_{i,m}|^2|)\Psi_{i,m}, \\ \partial_x \Psi_{i,m} &= \Phi_{i,m}. \end{aligned}$$

Figure 9: Multi-Symplectic Gauss-Legendre Collocation Methods for the Nonlinear Schrödinger Equation

In particular, the choice $r = s = 1$ leads again to a Preissmann scheme

$$\begin{aligned}
\frac{\mathrm{i}}{\Delta t}\left(\psi_{1/2}^{1} - \psi_{1/2}^{0}\right) &= \frac{1}{\Delta x}\left(\phi_{1}^{1/2} - \phi_{0}^{1/2}\right) + V'(|\psi_{1/2}^{1/2}|^2)\psi_{1/2}^{1/2}, \\
\frac{1}{\Delta x}\left(\psi_{1}^{1/2} - \psi_{0}^{1/2}\right) &= \phi_{1/2}^{1/2}
\end{aligned}$$

with

$$\psi_{1/2}^{m} = \frac{1}{2}\left(\psi_1^m + \psi_0^m\right), \quad \psi_i^{1/2} = \frac{1}{2}\left(\psi_i^1 + \psi_i^0\right), \quad \phi_i^{1/2} = \frac{1}{2}\left(\phi_i^1 + \phi_i^0\right),$$

$m, i = 1, 2$, and

$$\psi_{1/2}^{1/2} = \frac{1}{4}\left(\psi_1^1 + \psi_0^1 + \psi_1^0 + \psi_0^0\right), \quad \phi_{1/2}^{1/2} = \frac{1}{4}\left(\phi_1^1 + \phi_0^1 + \phi_1^0 + \phi_0^0\right).$$

We like to point out that any multi-symplectic Gauss-Legendre discretization will exactly preserve a discrete version of the conservation law (49). This follows from the quadratic form of the conservation law and the fact that quadratic conservation laws are exactly preserved by Gauss-Legendre methods.

When it comes to the integration of an initial-boundary value (Cauchy) problem, one could discretize in space using a Gauss-Legendre method and replace the temporal discretization by any convenient symplectic discretization of the spatially truncated system. Similar to what has been shown in §4 for the nonlinear wave equation, we would again obtain multi-symplectic methods.

7 Concluding Remarks

Theoretical results indicate [3, 4, 5] that the multi-symplectic structure of certain PDEs is crucial for a deeper understanding of wave phenomena. One of the nice features is that it is a strictly local concept and that it can be formulated as a conservation law involving differential two forms. It is thus also a very natural generalization of the conservation of symplecticity for canonical Hamiltonian systems. The results of this paper show that it is possible to find higher order multi-symplectic methods in a rather general setting again similar to the finite dimensional situation.

The suggested Gauss-Legendre discretizations for the one dimensional nonlinear wave equation (1) naturally generalize to any multi-symplectic PDE (2). Furthermore, they can also be applied to higher-dimensional nonlinear wave equations like, for example,

$$\partial_{tt}u - \partial_{xx}u - \partial_{yy}u = -V'(u)$$

and, more generally, to multi-symplectic PDEs like, for example,

$$\mathbf{M}\partial_t \boldsymbol{z} + \mathbf{K}\partial_x \boldsymbol{z} + \mathbf{L}\partial_y \boldsymbol{z} = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}).$$

This also implies that the schemes can be applied to the corresponding stationary problems characterised by $\partial_t \boldsymbol{z} = \mathbf{0}$.

Further results on multi-symplectic methods in the context of finite volume methods can be found in [17].

Acknowledgement. We like to thank Tom Bridges for the introduction to his framework of multi-symplectic PDEs and for many stimulating discussions during the preparation of this paper.

References

[1] M. B. ABBOTT & D. R. BASCO, *Computational Fluid Dynamics*, Longman Scientific & Technical, 1989.

[2] G. BENETTIN & A. GIORGILLI, *On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms*, J. Stat. Phys. **74** (1994) 1117–1143.

[3] TH. J. BRIDGES, *Multi-symplectic structures and wave propagation*, Math. Proc. Camb. Phil. Soc. **121** (1997) 147–190.

[4] TH. J. BRIDGES, *A geometric formulation of the conservation of wave action and its implications for signature and the classification of instabilities*, Proc. R. Soc. Lond. A **453** (1997), 1365–1395.

[5] TH. J. BRIDGES & G. DERKS, *Unstable eigenvalues, and the linearization about solitary waves and fronts with symmetry*, Proc. R. Soc. Lond. A (1999), to appear.

[6] TH. J. BRIDGES & S. REICH, *Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity*, technical report.

[7] G. J. COOPER, *Stability of Runge-Kutta methods for trajectory problems*, IMA J. Numer. Anal. **7** (1987), 1–13.

[8] D. B. DUNCAN, *Symplectic finite difference approximations of the nonlinear Klein-Gordon equation*, SIAM J. Numer. Anal. **34** (1997), 1742–1760.

[9] B. FORNBERG, *A Practical Guide to Pseudospectral Methods*, Cambridge University Press, 1998.

[10] S. JIMÉNEZ, *Derivation of the discrete conservation laws for a family of finite difference schemes*, Applied Mathematics and Computation **64** (1994), 13–45.

[11] J. E. MARSDEN, G. P. PATRICK & S. SHKOLLER, *Multisymplectic geometry, variational integrators, and nonlinear PDEs*, Comm. in Math. Phys., **199** (1999), 351-395.

[12] J. E. MARSDEN & S. SHKOLLER, *Multisymplectic geometry, covariant Hamiltonians and water waves*, Math. Proc. Camb. Phil. Soc. **125** (1999), 553–575.

[13] R. I. MCLACHLAN, *Symplectic integration of Hamiltonian wave equations*, Numer. Math. **66** (1994) 465–492.

[14] R. I. MCLACHLAN, *On the numerical integration of ordinary differential equations by symmetric composition methods*, SIAM J. Sci. Comput. **16** (1995), 151–168.

[15] S. LI & L. VU-QUOC, *Finite difference calculus invariant structure of a class of algorithms for the nonlinear Klein-Gordon equation*, SIAM J. Numer. Anal. **32** (1995), 1839–1875.

[16] S. REICH, *Backward error analysis for numerical integrators*, SIAM Numer. Anal. (1999) to appear.

[17] S. REICH, *Finite volume methods for multi-symplectic PDEs*, technical report, 1999.

[18] J. M. SANZ-SERNA & M. P. CALVO, *Numerical Hamiltonian Systems*, Chapman & Hall, London, 1994.

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

[20] A. P. Veselov, *Integrable discrete-time systems and difference operators*, Functs. Anal. Prilozhen. **22** (1988), 1–13.

[21] L. Vu-Quoc & S. Li, *Invariant-conserving finite difference algorithms for the nonlinear Klein-Gordon equation*, Computer Methods in Applied Mechanics and Engineering **107** (1993), 341–391.

Appendix: Energy Conserving Preissmann Scheme

The Preissmann scheme (35) applied to the wave equation (1) results in the system

$$\frac{u^1_{1/2}-u^0_{1/2}}{\Delta t} = \frac{v^1_{1/2}+v^0_{1/2}}{2}\,, \tag{50}$$

$$\frac{v^1_{1/2}-v^0_{1/2}}{\Delta t} = \frac{w^{1/2}_1-w^{1/2}_0}{\Delta x} - V'(u^{1/2}_{1/2})\,, \tag{51}$$

$$\frac{u^{1/2}_1-u^{1/2}_0}{\Delta x} = \frac{w^{1/2}_1+w^{1/2}_0}{2}\,. \tag{52}$$

Following Li & Vu-Quoc [21, 15], we modify the equation (51) to

$$\frac{v^1_{1/2}-v^0_{1/2}}{\Delta t} = \frac{w^{1/2}_1-w^{1/2}_0}{\Delta x} - \frac{V(u^1_{1/2})-V(u^0_{1/2})}{u^1_{1/2}-u^0_{1/2}}\,, \tag{53}$$

We like to show that this modified scheme exactly conserves the discrete energy conservation law

$$\frac{E^1_{1/2}-E^0_{1/2}}{\Delta t} + \frac{F^{1/2}_1-F^{1/2}_0}{\Delta x} = 0$$

with the abbreviations

$$E^n_{1/2} = \frac{1}{2}\left(\left(w^n_{1/2}\right)^2 + \left(v^n_{1/2}\right)^2\right) + V(u^n_{1/2}) \quad \text{and} \quad F^{1/2}_m = -v^{1/2}_m w^{1/2}_m\,,$$

$n, m = 0, 1$. This discrete energy conservation law corresponds to the formula (36) with $r = s = 1$, $b_1 = \tilde{b}_1 = 1$, and $i = m = 1/2$.

For the subsequent derivation it is crucial to observe that the solutions of (50)-(52) as well as of (50) and (52)-(53) satisfy

$$\frac{w^1_{1/2}-w^0_{1/2}}{\Delta t} = \frac{1}{\Delta t}\left(\frac{u^1_1-u^1_0}{\Delta x} - \frac{u^0_1-u^0_0}{\Delta x}\right) = \frac{1}{\Delta x}\left(\frac{u^1_1-u^0_1}{\Delta t} - \frac{u^1_0-u^0_0}{\Delta x}\right) = \frac{v^{1/2}_1-v^{1/2}_0}{\Delta x}\,.$$

We now premultiply (52) by $(w^1_{1/2}-w^0_{1/2})/\Delta t$ and use the above identity to obtain

$$\frac{\left(w^1_{1/2}\right)^2-\left(w^0_{1/2}\right)^2}{2\Delta t} = \frac{w^1_{1/2}-w^0_{1/2}}{\Delta t}\frac{u^{1/2}_1-u^{1/2}_0}{\Delta x} = \frac{v^{1/2}_1-v^{1/2}_0}{\Delta x}\frac{w^{1/2}_1+w^{1/2}_0}{2}\,. \tag{54}$$

Next we premultiply (50) by $(v^1_{1/2}-v^0_{1/2})/\Delta t$ which yields

$$\frac{\left(v^1_{1/2}\right)^2-\left(v^0_{1/2}\right)^2}{2\Delta t} = \frac{v^1_{1/2}-v^0_{1/2}}{\Delta t}\frac{u^1_{1/2}-u^0_{1/2}}{\Delta t}\,.$$

Finally, equation (53) is premultiplied by $(u^1_{1/2} - u^0_{1/2})/\Delta t$ which, using the previous equation, results in

$$\frac{\left(v^1_{1/2}\right)^2 - \left(v^0_{1/2}\right)^2}{2\Delta t} = \frac{v^1_{1/2} + v^0_{1/2}}{2} \frac{w^{1/2}_1 - w^{1/2}_0}{\Delta x} - \frac{V(u^1_{1/2}) - V(u^0_{1/2})}{\Delta t}\,. \tag{55}$$

Upon combining (54) and (55), we get

$$\begin{aligned} \frac{E^1_{1/2} - E^0_{1/2}}{\Delta t} &= \frac{v^{1/2}_1 + v^{1/2}_0}{2} \frac{w^{1/2}_1 - w^{1/2}_0}{\Delta x} + \frac{v^{1/2}_1 - v^{1/2}_0}{\Delta x} \frac{w^{1/2}_1 + w^{1/2}_0}{2} \\ &= \frac{v^{1/2}_1 w^{1/2}_1 - v^{1/2}_0 w^{1/2}_0}{\Delta x} \\ &= -\frac{F^{1/2}_1 - F^{1/2}_0}{\Delta x} \end{aligned}$$

as desired. The system (50) and (52)-(53) does not, in general preserve the momentum conservation law

$$\frac{I^1_{1/2} - I^0_{1/2}}{\Delta t} + \frac{G^{1/2}_1 - G^{1/2}_0}{\Delta t} = 0$$

with

$$I^n_{1/2} = -v^n_{1/2} w^n_{1/2} \quad \text{and} \quad G^{1/2}_m = \frac{1}{2}\left(\left(v^{1/2}_m\right)^2 + \left(w^{1/2}_m\right)^2\right) - V(u^{1/2}_m)\,.$$

To obtain a momentum conserving algorithm, (53) has to be replaced by

$$\frac{v^1_{1/2} - v^0_{1/2}}{\Delta t} = \frac{w^{1/2}_1 - w^{1/2}_0}{\Delta x} - \frac{V(u^{1/2}_1) - V(u^{1/2}_0)}{u^{1/2}_1 - u^{1/2}_0}\,.$$