Multi-Symplectic Integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity

Thomas J. Bridges and Sebastian Reich

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

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Abstract

The symplectic numerical integration of finite-dimensional Hamiltonian systems is a well established subject and has led to a deeper understanding of exisiting methods as well as to the development of new very efficient and accurate schemes, e.g., for rigid body, constrained, and molecular dynamics. The numerical integration of infinite-dimensional Hamiltonian systems or Hamiltonian PDEs is much less explored. In this paper, we suggest a new theoretical framework for generalizing symplectic numerical integrators for ODEs to Hamiltonian PDEs in $\mathbb{R}^2$: time plus one space dimension. The central idea is that symplecticity for Hamiltonian PDEs is directional: the symplectic structure of the PDE is decomposed into distinct components representing space and time independently. In this setting PDE integrators can be constructed by concatenating uni-directional ODE symplectic integrators. This suggests a natural definition of *multi-symplectic integrator* as a discretization that conserves a discrete version of the *conservation of symplecticity* for Hamiltonian PDEs. We show that this approach leads to a general framework for geometric numerical schemes for Hamiltonian PDEs, which have remarkable energy and momentum conservation properties. Generalizations, including development of higher-order methods, application to perturbed systems, and extension to more than one space dimension are also discussed.

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1 Introduction

The concept of a *symplectic integrator* has proven to be a very robust framework for the accurate, efficient and long-time integration of finite-dimensional Hamiltonian systems (see SANZ-SERNA & CALVO [17] for an overview and [9] for applications in the context of molecular dynamics). The basic idea of a symplectic integrator is that the numerical scheme is designed to preserve the symplectic form at each time step. For example, let $(\boldsymbol{q},\boldsymbol{p}) \in \mathrm{R}^{2n}$ be canonical coordinates and let $H : \mathrm{R}^{2n} \to \mathrm{R}$ be a smooth function. The continuous-time Hamiltonian system

$$\begin{aligned} \boldsymbol{q}_t &= +\boldsymbol{\nabla}_{\boldsymbol{p}} H(\boldsymbol{q},\boldsymbol{p}), &(1.1)\\ \boldsymbol{p}_t &= -\boldsymbol{\nabla}_{\boldsymbol{q}} H(\boldsymbol{q},\boldsymbol{p}), &(1.2)\end{aligned}$$

preserves exactly the symplectic form

$$\boldsymbol{\omega} = \boldsymbol{dp} \wedge \boldsymbol{dq} = \boldsymbol{dp}^T \boldsymbol{dq} - \boldsymbol{dq}^T \boldsymbol{dp}\,; \qquad (1.3)$$

that is,

$$\frac{d\boldsymbol{\omega}}{dt} = \boldsymbol{dp}_t \wedge \boldsymbol{dq} + \boldsymbol{dp} \wedge \boldsymbol{dq}_t = 0\,, \qquad (1.4)$$

where $\boldsymbol{dq}, \boldsymbol{dp} \in \mathrm{R}^{n\times 2n}$ are solutions of the matrix-valued *variational equation*

$$\begin{aligned} \boldsymbol{dq}_t &= +\boldsymbol{D}_{\boldsymbol{qq}} H(\boldsymbol{q},\boldsymbol{p})\boldsymbol{dq} + \boldsymbol{D}_{\boldsymbol{qp}} H(\boldsymbol{q},\boldsymbol{p})\boldsymbol{dp}, &(1.5)\\ \boldsymbol{dp}_t &= -\boldsymbol{D}_{\boldsymbol{pq}} H(\boldsymbol{q},\boldsymbol{p})\boldsymbol{dq} - \boldsymbol{D}_{\boldsymbol{pp}} H(\boldsymbol{q},\boldsymbol{p})\boldsymbol{dp}\,. &(1.6)\end{aligned}$$

A symplectic integrator is a numerical approximation for (1.1)-(1.3)

$$\boldsymbol{z}_{j+1} = \boldsymbol{\Psi}_{\Delta t}(\boldsymbol{z}_j)\,, \quad \boldsymbol{z}_j = (\boldsymbol{q}_j, \boldsymbol{p}_j)\,, \quad t_{j+1} = t_j + \Delta t\,, \qquad (1.7)$$

whose linearization $\boldsymbol{dz}_{j+1} = \boldsymbol{D}_{\boldsymbol{z}}\boldsymbol{\Psi}_{\Delta t}(\boldsymbol{z}_j)\boldsymbol{dz}_j$ respects a discrete approximation of (1.4):

$$\frac{\boldsymbol{\omega}_{j+1} - \boldsymbol{\omega}_j}{\Delta t} = \frac{\boldsymbol{dp}_{j+1} \wedge \boldsymbol{dq}_{j+1} - \boldsymbol{dp}_j \wedge \boldsymbol{dq}_j}{\Delta t} = 0\,, \qquad (1.8)$$

or

$$\boldsymbol{dp}_{j+1} \wedge \boldsymbol{dq}_{j+1} = \boldsymbol{dp}_j \wedge \boldsymbol{dq}_j\,. \qquad (1.9)$$

This conservation property of a symplectic integrator gives rise to excellent long time behaviour which can be explained in terms of backward error analysis (see, for example, [3, 15]).

For generalization to PDEs it is useful to abstract (1.1)-(1.3) as follows. Let $\mathbf{J}$ be any skew-symmetric invertible matrix on $\mathbb{R}^{2n}$. Then $(\mathbb{R}^{2n}, \boldsymbol{\omega})$ is a symplectic manifold with $\boldsymbol{\omega}(U,V) = \langle \mathbf{J}U, V\rangle$ where $U, V \in \mathbb{R}^{2n}$ and $\langle\cdot,\cdot\rangle$ is the standard inner product on $\mathbb{R}^{2n}$. A (autonomous) Hamiltonian system on this symplectic structure takes the form

$$\mathbf{J}\boldsymbol{z}_t = \boldsymbol{\nabla}_{\boldsymbol{z}} H(\boldsymbol{z})\,, \quad \boldsymbol{z} \in \mathbb{R}^{2n}\,, \qquad (1.10)$$

with the two attendant conservation laws

$$\frac{d}{dt}\boldsymbol{\omega} = 0 \quad \text{and} \quad \frac{d}{dt} H(\boldsymbol{z}) = 0\,. \qquad (1.11)$$

The first conservation law is conservation of symplecticity and the second is conservation of energy.

The most obvious generalization of the concept of a symplectic integrator to Hamiltonian PDEs is a numerical scheme which is designed to preserve a semi-discretization of the symplectic form associated with the infinite-dimensional evolution equation. For example, consider the non-linear wave equation

$$u_{tt} - u_{xx} + V'(u) = 0\,, \qquad (1.12)$$

where $V(u)$ is some smooth function and u is scalar valued. By defining a new variable $v = u_t$, this system can be written as a canonical – infinite-dimensional – Hamiltonian system

$$\begin{aligned} u_t &= +\frac{\delta H}{\delta v} = v\,, &(1.13)\\ v_t &= -\frac{\delta H}{\delta u} = u_{xx} - V'(u)\,, &(1.14)\end{aligned}$$

where

$$H(u,v) = \int_0^L [\, \tfrac{1}{2}v^2 + \tfrac{1}{2}u_x^2 + V(u)\,]\, dx\,, \tag{1.15}$$

and L is the length of the spatial domain. The symplectic form for this system is

$$\overline{\boldsymbol{\omega}} = \int_0^L \boldsymbol{d}v \wedge \boldsymbol{d}u \, dx \tag{1.16}$$

where the overbar on $\overline{\boldsymbol{\omega}}$ is a reminder that the two-form $\boldsymbol{d}v \wedge \boldsymbol{d}u$ is integrated over all space. A semi-discretization of this system leads to system of ODEs which – if the semi-discretization is chosen properly – is a system of Hamiltonian ODEs with symplectic form given by a discrete version of (1.16). An overview of this point of view in terms of symplectic time-integration methods is given by MacLachlan [14].

The problem with this approach to developing a symplectic integrator for PDEs is that it is global. In other words, by integrating (summing) over the total $x-$domain, local variations in symplecticity are averaged, and there may be anomalies in the spatial distribution of symplecticity that are masked by averaging. A more satisfactory approach is to develop a *local concept of symplecticity* for Hamiltonian PDEs, since – in stark contrast to Hamiltonian ODEs – symplecticity may vary from point to point and from time to time, much like vorticity in a fluid flow.

Strip away the integral from $\overline{\boldsymbol{\omega}}$ in (1.16) and define $\boldsymbol{\omega} = \boldsymbol{d}v \wedge \boldsymbol{d}u$. Then

$$\frac{\partial}{\partial t}\boldsymbol{\omega} = \boldsymbol{d}v_t \wedge \boldsymbol{d}u + \boldsymbol{d}v \wedge \boldsymbol{d}u_t\,. \tag{1.17}$$

The forms $\boldsymbol{d}u$ and $\boldsymbol{d}v$ satisfy the *variational equation*

$$\begin{aligned} \boldsymbol{d}u_t &= \boldsymbol{d}v\,, && (1.18)\\ \boldsymbol{d}v_t &= \boldsymbol{d}u_{xx} - V''(u)\boldsymbol{d}u\,. && (1.19) \end{aligned}$$

Substituting terms from the variational equations into (1.17) leads to

$$\begin{aligned} \frac{\partial}{\partial t}\boldsymbol{\omega} &= (\boldsymbol{d}u_{xx} - V''(u)\boldsymbol{d}u) \wedge \boldsymbol{d}u + \boldsymbol{d}v \wedge \boldsymbol{d}v\,, && (1.20)\\ &= \boldsymbol{d}u_{xx} \wedge \boldsymbol{d}u = \frac{\partial}{\partial x}(\boldsymbol{d}u_x \wedge \boldsymbol{d}u)\,. && (1.21) \end{aligned}$$

Let $w = u_x$ and $\boldsymbol{\kappa} = \boldsymbol{d}u \wedge \boldsymbol{d}w$. Then $(\boldsymbol{\omega}, \boldsymbol{\kappa})$ satisfy *conservation of symplecticity*

$$\frac{\partial}{\partial t}\boldsymbol{\omega} + \frac{\partial}{\partial x}\boldsymbol{\kappa} = 0\,, \tag{1.22}$$

(cf. [5, 6]). Not only is this equation local, it emphasizes a fundamental aspect of symplecticity for Hamiltonian PDEs: it varies over a spatial domain; one can talk about regions of "low symplecticity" and "high symplecticity" and one can think of $\boldsymbol{\kappa}$ as representing "flux of symplecticity". A control volume formulation of (1.22) is

$$\oint (\boldsymbol{\omega}\, dx - \boldsymbol{\kappa}\, dt) = 0 \tag{1.23}$$

where the integral is over any closed contour in a simply-connected subset of the (x,t)-plane.

This approach to Hamiltonian PDEs can be abstracted as follows. Let $\mathbf{M}$ and $\mathbf{K}$ be *any* skew-symmetric matrices on $\mathbb{R}^n$ $(n \geq 3)$ and let $S : \mathbb{R}^n \to \mathbb{R}$ be *any* smooth function. Then, we will call a system of the following form a *Hamiltonian system on a multi-symplectic structure*,

$$\mathbf{M}\boldsymbol{z}_t + \mathbf{K}\boldsymbol{z}_x = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z})\,, \quad \boldsymbol{z} \in \mathbb{R}^n\,, \tag{1.24}$$

where the gradient $\boldsymbol{\nabla}_{\boldsymbol{z}}$ is defined with respect to the standard inner product on $\mathbb{R}^n$, denoted by $\langle \cdot, \cdot \rangle$. Note that there is no assumption in (1.24) that the equation is well-posed as an initial-value problem. Indeed, this formulation includes elliptic PDEs as well (see §3). The form of the equations (1.24) is interesting for two reasons: it is a natural generalization of (1.10) and a large class of PDEs can be formulated this way (cf. [5, 6, 8] for a multitude of examples: generalized KdV, nonlinear

Schrödinger models, Boussinesq models, geostrophic flow, water waves, Swift-Hohenberg equation, etc.). We now show that the natural generalization of $\boldsymbol{\omega}_t = 0$ in (1.11) is (1.22).

The system (1.24) is multi-symplectic in the following sense. Associated with $\mathbf{M}$ and $\mathbf{K}$ are the pre-symplectic forms

$$\boldsymbol{\omega}(U,V) = \langle \mathbf{M}U, V\rangle \quad \text{and} \quad \boldsymbol{\kappa}(U,V) = \langle \mathbf{K}U, V\rangle\,, \quad U,V \in \mathbb{R}^n\,. \tag{1.25}$$

The two-form $\boldsymbol{\omega}$ defines a symplectic structure on $\mathbb{R}^m$ $(m = \operatorname{rank}\mathbf{M} \le n)$ which is associated with the time direction and the two form $\boldsymbol{\kappa}$ defines a symplectic structure on $\mathbb{R}^k$ $(k = \operatorname{rank}\mathbf{K} \le n)$ which is associated with the $x-$direction.

Any system of the form (1.24) satisfies conservation of symplecticity. Let $U,V \in \mathbb{R}^n$ be any solutions of the variational equation associated with (1.24),

$$\mathbf{M}\boldsymbol{d}\boldsymbol{z}_t + \mathbf{K}\boldsymbol{d}\boldsymbol{z}_x = \boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z})\boldsymbol{d}\boldsymbol{z}\,. \tag{1.26}$$

Then

$$\begin{aligned} \frac{\partial}{\partial t}\boldsymbol{\omega} &= \langle \mathbf{M}U_t, V\rangle + \langle \mathbf{M}U, V_t\rangle & (1.27)\\ \frac{\partial}{\partial x}\boldsymbol{\kappa} &= \langle \mathbf{K}U_x, V\rangle + \langle \mathbf{K}U, V_x\rangle\,, & (1.28) \end{aligned}$$

and so

$$\begin{aligned} \partial_t\boldsymbol{\omega} + \partial_x\boldsymbol{\kappa} &= \langle \mathbf{M}U_t + \mathbf{K}U_x, V\rangle - \langle U, \mathbf{M}V_t + \mathbf{K}V_x\rangle & (1.29)\\ &= \langle \boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z})U, V\rangle - \langle U, \boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z})V\rangle & (1.30)\\ &= 0\,, & (1.31) \end{aligned}$$

since $\boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z})$ is a symmetric matrix.

Multi-symplectic systems of the form (1.24) were introduced in BRIDGES [5, 6]. There is an interesting connection between this formulation of Hamiltonian PDEs and the theory based on the Cartan form in field theory. MARSDEN & SHKOLLER [12] show that the collection of two forms can be concatenated into a single higher order form which is equivalent to the *exterior derivative* of the Cartan form in field theory. A sketch of this theory is as follows. Enlarge the manifold to the *extended phase space* $\mathbb{R}^n \times \mathbb{R}^s$ (where s is the dimension of space-time). Then, for the case considered in this paper where $s = 2$, the exterior derivative of the Cartan form is

$$\boldsymbol{\Omega} = \boldsymbol{\omega} \wedge \boldsymbol{d}x - \boldsymbol{\kappa} \wedge \boldsymbol{d}t - \boldsymbol{d}S \wedge \boldsymbol{d}x \wedge \boldsymbol{d}t \in \textstyle\bigwedge^3(\mathbb{R}^n \times \mathbb{R}^2)\,. \tag{1.32}$$

In field theory this $3-$form (or more generally $(s+1)-$form) is also called a multi-symplectic form (cf. BINZ ET AL. [4], page 330), but a natural name for this form is a *meta-symplectic form*. Essentially, the Cartan form – or meta-symplectic form – provides an invariantive setting for Hamiltonian PDEs. Given any vector field on the extended phase space, the governing equations are deduced by restricting $\boldsymbol{\Omega}$ to the image of a section (cf. [12] for details). For an elementary and historical account of the role of the Cartan form in field theory see KIJOWSKI & TULCZYJEW ([10], §20). In fact another approach to the development of numerical schemes is to start with a Lagrangian setting and preserve a discrete version of the Cartan form (cf. MARSDEN, PATRICK & SHKOLLER [11]). The Lagrangian formulation leads to an elegant generalization of VESELOV [13] sequences to Lagrangian PDEs. We will compare some aspects of this Lagrangian approach with the Hamiltonian setting proposed here in §3.

The approach proposed in this paper for numerical integration of Hamiltonian PDEs is modelled on the framework for Hamiltonian ODEs – indeed it has been shown in REICH [16] that higher-order symplectic integrators such as Gauss-Legendre Runge-Kutta methods can be generalized to multi-symplectic PDEs. We argue that the natural generalization of (1.10) is (1.24) and the natural generalization of (1.11) is (1.22). *Moreover the "phase space" for (1.24) is finite-dimensional so many of the ideas from ODEs carry over in a straightforward way.* This approach is particularly effective in overcoming the intrinsic limitations of discrete Lagrangian formulations such as restricted order. We will also show that the generalization of $\frac{d}{dt}H = 0$ in (1.11) is conservation of energy *and* momentum. We say that a numerical scheme is a *multi-symplectic integrator* if the numerical scheme preserves a discrete version of conservation of symplecticity.

An important property of symplectic integrators for Hamiltonian ODEs is that – when well designed – they show remarkable energy preserving properties. A natural question is how well multi-symplectic schemes for Hamiltonian PDEs conserve energy. Here we encounter the global-local question again. For example, the energy for the nonlinear wave equation (1.12) is the Hamiltonian function (1.15). After semi-discretization, the integral over x becomes a sum, and it is natural to enquire whether this total energy is conserved by an integrator. However, this is highly unsatisfactory: an integral (sum) over space can mask massive anomalies in the distribution of energy over space. A local concept of energy conservation is needed: a conservation law for energy. Moreover, in the space-time setting, when the Hamiltonian function S does not depend explicitly on x and t there are two fundamental conservation laws: in addition to conservation of energy, we have conservation of momentum.

For systems in the abstract form (1.24) there is a natural geometric form for energy and momentum conservation

$$\partial_t E(z) + \partial_x F(z) = 0 \quad \text{and} \quad \partial_t I(z) + \partial_x G(z) = 0\,, \tag{1.33}$$

where

$$E(z) \;=\; S(z) - \tfrac{1}{2}\boldsymbol{\kappa}(z_x, z)\,, \quad F(z) = \tfrac{1}{2}\boldsymbol{\kappa}(z_t, z)\,, \tag{1.34}$$

$$G(z) \;=\; S(z) - \tfrac{1}{2}\boldsymbol{\omega}(z_t, z)\,, \quad I(z) = \tfrac{1}{2}\boldsymbol{\omega}(z_x, z)\,. \tag{1.35}$$

(cf. [5]). Integrating the densities $E(z)$ and $I(z)$ over the spatial domain – with suitable boundary conditions – leads to (global) conserved quantites:

$$\frac{d}{dt}\mathcal{E}(z) = 0 \quad \text{and} \quad \frac{d}{dt}\mathcal{I}(z)\,, \tag{1.36}$$

where $\mathcal{E}(z) = \int_0^L E(z)\,dx$ and $\mathcal{I}(z) = \int_0^L I(z)\,dx$. Global conservation of energy or momentum (1.36) is a necessary but not sufficient condition for local conservation of energy or momentum (1.33). We will show in §5 that multi-symplectic schemes have remarkable *local* conservation – of both energy and momentum – over long time intervals.

An outline of the paper is as follows. In §2 we introduce discrete and continuous conservation of symplecticity and define a multi-symplectic integrator. In §3 we consider a canonical example of a semi-linear elliptic/hyperbolic PDE which includes (1.12) as a special case and has an interesting multi-symplectic structure on $\mathbb{R}^4$ with *both* $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}$ non-degenerate. We show that the most natural staggered box scheme for this system, obtained by concatenating two Störmer-Verlet/leapfrog schemes, is multi-symplectic. In §4 we consider abstract systems of the form (1.24) and show that the box scheme is multi-symplectic. In §5 we consider conservation of energy and momentum and show that multi-symplectic schemes show promising energy-momentum conservation properties. In §6 we discuss global properties of multi-symplectic schemes: a multi-symplectic scheme can be summed over the spatial index, leading to a Hamiltonian ODE with a classical symplectic structure. In the concluding remarks (§7) we discuss generalizations: higher space dimension; higher-order methods; other classical Hamiltonian PDEs with a multi-symplectic structure; and perturbed multi-symplectic systems.

2 Discrete conservation of symplecticity and multi-symplectic integrators

The starting point for the numerical framework is the following abstract formulation of Hamiltonian PDEs

$$\mathbf{M} z_t + \mathbf{K} z_x = \boldsymbol{\nabla}_z S(z)\,, \quad z \in \mathbb{R}^n\,, \quad (x,t) \in \mathbb{R}^2\,. \tag{2.1}$$

The basic hypotheses on this abstract form are that $\mathbf{M}$ and $\mathbf{K}$ are skew-symmetric matrices on $\mathbb{R}^n$, $n \geq 3$, and $S : \mathbb{R}^n \to \mathbb{R}$ is a smooth function (at least twice continuously differentiable). The gradient of S is with respect to an inner product on $\mathbb{R}^n$ which will be denoted by $\langle\cdot,\cdot\rangle$ throughout. Associated with (2.1) are the pair of differential two forms defined by

$$\boldsymbol{\omega}(U,V) = \langle \mathbf{M}U, V\rangle \quad \text{and} \quad \boldsymbol{\kappa}(U,V) = \langle \mathbf{K}U, V\rangle \quad \text{for any } U,V \in \mathbb{R}^n\,. \tag{2.2}$$

A fundamental geometric property of systems of the form (2.1) is that they conserve symplecticity:

$$\frac{\partial}{\partial t}\boldsymbol{\omega}(U,V) + \frac{\partial}{\partial x}\boldsymbol{\kappa}(U,V) = 0\,, \tag{2.3}$$

where U and V are *any pair* of solutions of the variational equation associated with (2.1) (cf. [6]).

$$\boldsymbol{M}\boldsymbol{dz}_t + \boldsymbol{K}\boldsymbol{dz}_x = \boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z})\boldsymbol{dz}\,, \quad \boldsymbol{dz} \in \mathbb{R}^n\,. \tag{2.4}$$

Given any closed contour $\mathcal{C}$ in a simply-connected subset of the (x,t)-plane, (2.3) is equivalent to

$$\oint_{\mathcal{C}} (\boldsymbol{\omega}\,dx - \boldsymbol{\kappa}\,dt) = 0\,. \tag{2.5}$$

The idea is to develop a numerical scheme for approximating (2.1) which also conserves a discrete analog of conservation of symplecticity. A numerical discretization of (2.1) can be written schematically as

$$\mathbf{M}\partial_t^{i,j}\boldsymbol{z}_{i,j} + \mathbf{K}\partial_x^{i,j}\boldsymbol{z}_{i,j} = (\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z}_{i,j}))_{i,j}\,, \quad \text{where} \quad \boldsymbol{z}_{i,j} = \boldsymbol{z}(x_i,t_j)\,, \tag{2.6}$$

and $\partial_t^{i,j}$ and $\partial_x^{i,j}$ are discretizations of the derivatives ∂_t and ∂_x respectively. A discrete version of the conservation of symplecticity – using the same discretization as in (2.6) – can be written schematically as follows

$$\partial_t^{i,j}\boldsymbol{\omega}_{i,j} + \partial_x^{i,j}\boldsymbol{\kappa}_{i,j} = 0\,, \tag{2.7}$$

where

$$\boldsymbol{\omega}_{i,j} = \langle \boldsymbol{M}U_{i,j}, V_{i,j}\rangle \quad \text{and} \quad \boldsymbol{\kappa}_{i,j} = \langle \boldsymbol{K}U_{i,j}, V_{i,j}\rangle\,,$$

and $\{U_{i,j}\}_{(i,j)\in\mathbb{Z}\times\mathbb{Z}}$ and $\{V_{i,j}\}_{(i,j)\in\mathbb{Z}\times\mathbb{Z}}$ satisfy the *discrete variational equations*

$$\mathbf{M}\partial_t^{i,j}\boldsymbol{dz}_{i,j} + \mathbf{K}\partial_x^{i,j}\boldsymbol{dz}_{i,j} = \boldsymbol{D}_{\boldsymbol{zz}}^{i,j}S(\boldsymbol{z}_{i,j})\boldsymbol{dz}_{i,j}\,. \tag{2.8}$$

Definition. *The numerical scheme (2.6) is called a multi-symplectic integrator if (2.7) is a discrete conservation law for (2.6).*

In the next two sections, examples of multi-symplectic integrators are given. In the remainder of this section, we give some indication of how well-known Hamiltonian PDEs can be formulated in the abstract form (2.1).

Many conservative PDEs can be written in the form (2.1): nonlinear wave equations (see §3), shallow-water equations, atmospheric flows, fluid-structure interaction, water waves, KdV equation, KP equation and nonlinear Schrödinger models (cf. [5], [6]). Multi-symplectifications of NLS models and gKdV are constructed as follows. First consider the following class of nonlinear Schrödinger models

$$i\Psi_t = \Psi_{xx} + V'(|\Psi|^2)\Psi\,, \quad (x,t)\in\mathbb{R}^2\,, \quad \Psi\in\mathbb{C}\,, \tag{2.9}$$

where $V:\mathbb{R}\to\mathbb{R}$ is any given smooth function [8]. With $\Psi = q_1 + iq_2$ and $\Psi_x = p_1 + ip_2$, (2.9) has the multi-symplectic representation (2.1) with the matrices $\mathbf{M}$ and $\mathbf{K}$ defined by

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

$\boldsymbol{z} = (q_1, q_2, p_1, p_2)^T$, and

$$S(\boldsymbol{z}) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}V(q_1^2 + q_2^2)\,.$$

Another example is provided by the generalized Korteweg-de Vries (gKdV) equation, written in Hamiltonian form,

$$u_t = -\frac{1}{2}\frac{\partial}{\partial x}\frac{\partial H}{\partial u}, \quad \text{with} \quad H(u) = \int_{-\infty}^{+\infty}\left[V(u) - \frac{1}{2}u_x^2\right]dx,$$

where $V(u)$ is some smooth function. The gKdV equation can be reformulated as a Hamiltonian system on a multi-symplectic structure as follows [8]. With new variables, ϕ, v, and w, defined below, the gKdV equation becomes a first-order system of PDEs,

$$u = \phi_x, \quad v = u_x, \quad w = \phi_t + v_x + V'(u), \quad u_t + w_x = 0,$$

or with $\boldsymbol{z} = (\phi, u, v, w)^T \in \mathbb{R}^4$,

$$\mathbf{M}\boldsymbol{z}_t + \mathbf{K}\boldsymbol{z}_x = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}) \tag{2.10}$$

where

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

and

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

3 Semilinear wave equations and a staggered multi-symplectic leapfrog scheme

Natural mechanical systems in a finite-dimensional space, where the Hamiltonian function consists of a sum of kinetic and potential energies,

$$H(\boldsymbol{q}, \boldsymbol{p}) = \tfrac{1}{2}\boldsymbol{p}^T \boldsymbol{B}^{-1}\boldsymbol{p} + V(\boldsymbol{q}), \qquad (\boldsymbol{q}, \boldsymbol{p}) \in \mathbb{R}^{2n},$$

are often discretized by the *staggered Störmer-Verlet scheme*

$$\boldsymbol{q}_{j+1} = \boldsymbol{q}_j + \Delta t\, \boldsymbol{B}^{-1}\boldsymbol{p}_{j+\frac{1}{2}}, \tag{3.1}$$

$$\boldsymbol{p}_{j+\frac{1}{2}} = \boldsymbol{p}_{j-\frac{1}{2}} - \Delta t\, \boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q}_j) \tag{3.2}$$

where $(\boldsymbol{q}_j, \boldsymbol{p}_j) = (\boldsymbol{q}(t_j), \boldsymbol{p}(t_j))$ and $t_j = t_0 + j\Delta t$. This scheme is symplectic with respect to a staggered wedge product. Let

$$\boldsymbol{\omega}_j = \boldsymbol{dq}_j \wedge \boldsymbol{dp}_{j+\frac{1}{2}},$$

where $\boldsymbol{dq}_j$ and $\boldsymbol{dp}_{j+\frac{1}{2}}$ are solutions of the discrete variational equation associated with (3.1); then

$$\frac{\boldsymbol{\omega}_{j+1} - \boldsymbol{\omega}_j}{\Delta t} = 0,$$

or, $\boldsymbol{\omega}_{j+1} = \boldsymbol{\omega}_j$ (cf. [17]).

In this section, we give a simple example of a multi-symplectic integrator by concatenating a staggered Störmer-Verlet scheme in the $x-$direction and the $t-$direction. Consider the following canonical model Hamiltonian PDE: the semilinear hyperbolic/elliptic scalar PDE:

$$u_{tt} + \varepsilon u_{xx} + V'(u) = 0, \quad \varepsilon = \pm 1. \tag{3.3}$$

The function $u(x,t)$ is scalar valued and $V(u)$ is some smooth potential function. When $\varepsilon = +1$ this PDE is elliptic and when $\varepsilon = -1$ it is hyperbolic.

A first-order system of PDEs equivalent to (3.3) is

$$v_t + w_x + V'(u) = 0 \tag{3.4}$$

$$v = u_t + p_x \tag{3.5}$$

$$w = \varepsilon u_x - p_t \tag{3.6}$$

$$\varepsilon w_t - v_x = 0. \tag{3.7}$$

The additional variable $p(x,t)$ is essentially a Lagrange multiplier associated with the constraint $\varepsilon w_t - v_x = 0$, much like the pressure in the Euler equations in fluid mechanics. The system (3.4) can be written in the abstract form (2.1) by taking

$$\mathbf{M} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\varepsilon \\ 0 & 0 & \varepsilon & 0 \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, \tag{3.8}$$

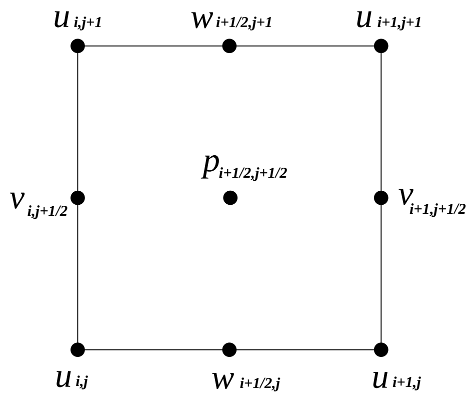

Figure 1: Schematic of the staggered mesh

and

$$S(z) = \tfrac{1}{2}(v^2 + \varepsilon w^2) + V(u)\,, \quad \text{with} \quad z = \begin{pmatrix} u \\ v \\ w \\ p \end{pmatrix} \in \mathbb{R}^4\,. \tag{3.9}$$

The pair of differential two forms which define the multi-symplectic structure are

$$\boldsymbol{\omega} = \boldsymbol{d}v \wedge \boldsymbol{d}u + \varepsilon \boldsymbol{d}p \wedge \boldsymbol{d}w \quad \text{and} \quad \boldsymbol{\kappa} = \boldsymbol{d}w \wedge \boldsymbol{d}u + \boldsymbol{d}v \wedge \boldsymbol{d}p\,. \tag{3.10}$$

The scalar PDE (3.3) – for both the elliptic and hyperbolic cases – is completely characterized by the pair of differential two forms $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}$ and the scalar-valued function S defined in (3.9). Note that both $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}$ are non-degenerate on the full phase space, $\mathbb{R}^4$.

A natural discretization of the system (3.4) is a staggered box scheme, constructed by concatenating two copies of the staggered leapfrog scheme. The values of u are placed at the corners of the box, v and w are at the centre of the edges and p is in the centre of the box, as shown in Figure 3.1.

This layout of the mesh and the field variables leads immediately to the following discrete system

$$\begin{aligned}
-\frac{v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}}{\Delta t} - \frac{w_{i+\frac{1}{2},j} - w_{i-\frac{1}{2},j}}{\Delta x} &= V'(u_{i,j}) && (3.11)\\
\frac{u_{i,j+1} - u_{i,j}}{\Delta t} + \frac{p_{i+\frac{1}{2},j+\frac{1}{2}} - p_{i-\frac{1}{2},j+\frac{1}{2}}}{\Delta x} &= v_{i,j+\frac{1}{2}} && (3.12)\\
\frac{u_{i+1,j} - u_{i,j}}{\Delta x} - \varepsilon\,\frac{p_{i+\frac{1}{2},j+\frac{1}{2}} - p_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta t} &= \varepsilon\, w_{i+\frac{1}{2},j} && (3.13)\\
\varepsilon\,\frac{w_{i+\frac{1}{2},j+1} - w_{i+\frac{1}{2},j}}{\Delta t} - \frac{v_{i+1,j+\frac{1}{2}} - v_{i,j+\frac{1}{2}}}{\Delta x} &= 0\,. && (3.14)
\end{aligned}$$

We will prove two results about this discretization: it is multi-symplectic and secondly – when $\varepsilon = -1$ – it is precisely a multi-symplectification of the classical leapfrog scheme for nonlinear wave equations. When $\varepsilon = +1$, it is the elliptic equivalent of the leapfrog discretization; the symmetric centred difference scheme for the Laplacian and Poisson equations.

To prove that the above staggered discretization is multi-symplectic we need the discrete variational equations associated with (3.11)-(3.14):

$$\begin{aligned}
-\frac{\boldsymbol{d}v_{i,j+\frac{1}{2}} - \boldsymbol{d}v_{i,j-\frac{1}{2}}}{\Delta t} - \frac{\boldsymbol{d}w_{i+\frac{1}{2},j} - \boldsymbol{d}w_{i-\frac{1}{2},j}}{\Delta x} &= V''(u_{i,j})\boldsymbol{d}u_{i,j}\\
\frac{\boldsymbol{d}u_{i,j+1} - \boldsymbol{d}u_{i,j}}{\Delta t} + \frac{\boldsymbol{d}p_{i+\frac{1}{2},j+\frac{1}{2}} - \boldsymbol{d}p_{i-\frac{1}{2},j+\frac{1}{2}}}{\Delta x} &= \boldsymbol{d}v_{i,j+\frac{1}{2}}\\
\frac{\boldsymbol{d}u_{i+1,j} - \boldsymbol{d}u_{i,j}}{\Delta x} - \varepsilon\,\frac{\boldsymbol{d}p_{i+\frac{1}{2},j+\frac{1}{2}} - \boldsymbol{d}p_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta t} &= \varepsilon\, \boldsymbol{d}w_{i+\frac{1}{2},j}\\
\varepsilon\,\frac{\boldsymbol{d}w_{i+\frac{1}{2},j+1} - \boldsymbol{d}w_{i+\frac{1}{2},j}}{\Delta t} - \frac{\boldsymbol{d}v_{i+1,j+\frac{1}{2}} - \boldsymbol{d}v_{i,j+\frac{1}{2}}}{\Delta x} &= 0\,.
\end{aligned}$$

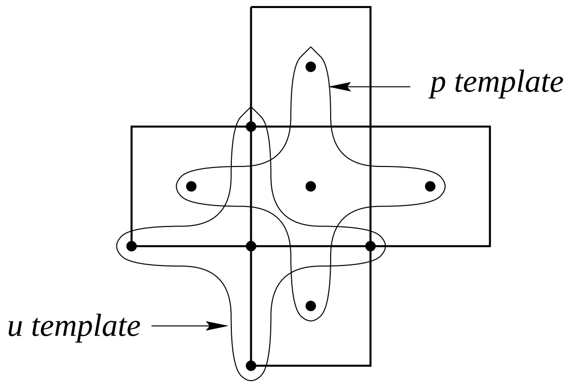

Figure 2: Template for staggered leapfrog in configuration space

Based on the definitions of $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}$ in (3.10) we defined the staggered discrete two forms

$$\boldsymbol{\omega}_{i,j} = \boldsymbol{d}v_{i,j-\frac{1}{2}} \wedge \boldsymbol{d}u_{i,j} + \varepsilon \boldsymbol{d}p_{i+\frac{1}{2},j-\frac{1}{2}} \wedge \boldsymbol{d}w_{i+\frac{1}{2},j}\,, \tag{3.15}$$

and

$$\boldsymbol{\kappa}_{i,j} = \boldsymbol{d}w_{i-\frac{1}{2},j} \wedge \boldsymbol{d}u_{i,j} + \boldsymbol{d}v_{i,j+\frac{1}{2}} \wedge \boldsymbol{d}p_{i-\frac{1}{2},j+\frac{1}{2}}\,. \tag{3.16}$$

Proposition. *The above staggered mesh discretization for (3.3) is a multi-symplectic integrator. Let $\boldsymbol{\omega}_{i,j}$ and $\boldsymbol{\kappa}_{i,j}$ be as defined in (3.15) and (3.16) respectively. Then, when evaluated on solutions of the discrete variational equation (4.8), these two forms satisfy*

$$\frac{\boldsymbol{\omega}_{i,j+1} - \boldsymbol{\omega}_{i,j}}{\Delta t} + \frac{\boldsymbol{\kappa}_{i+1,j} - \boldsymbol{\kappa}_{i,j}}{\Delta x} = 0\,. \tag{3.17}$$

The proof is a straightforward calculation using the discrete variational equation and the definitions of the staggered two-forms $\boldsymbol{\omega}_{i,j}$ and $\boldsymbol{\kappa}_{i,j}$.

In addition to being a natural concatenation of the symplectic Störmer-Verlet scheme, this staggered multi-symplectic scheme is also a reformulation of the classical leapfrog discretization for the wave equation (when $\varepsilon = -1$, with the analogue for elliptic equations when $\varepsilon = +1$). To see this, substitute $v_{i,j+\frac{1}{2}}$ and $w_{i+\frac{1}{2},j}$ into the equations (3.11) and (3.14). These substitutions lead to

$$\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta t^2} + \varepsilon\,\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + V'(u_{i,j}) = 0\,, \tag{3.18}$$

and

$$\begin{aligned}&\frac{p_{i+\frac{1}{2},j+\frac{3}{2}} - 2p_{i+\frac{1}{2},j+\frac{1}{2}} + p_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta t^2}\\ &\qquad + \varepsilon\,\frac{p_{i+\frac{3}{2},j+\frac{1}{2}} - 2p_{i+\frac{1}{2},j+\frac{1}{2}} + p_{i-\frac{1}{2},j+\frac{1}{2}}}{\Delta x^2} = 0\,.\end{aligned} \tag{3.19}$$

When $\varepsilon = -1$ the system decouples into two leapfrog discretizations for $u_{i,j}$ and $p_{i,j}$ respectively, and when $\varepsilon = +1$ it is a pair of symmetric centred-difference schemes for elliptic equations with the Laplacian as main part; see Figure 3.2.

It is important to note that the discretization and the method of solution of the complete set of difference equations are two distinct issues. For example, the above discretization will require dramatically different solution techniques for the two cases $\varepsilon = -1$ and $\varepsilon = +1$. When $\varepsilon = -1$ a sweep technique is possible, whereas when $\varepsilon = +1$ all mesh points are coupled due to ellipticity and a global solver is necessary.

We now compare our formulation of a multi-symplectic scheme with the multi-symplectic framework proposed by Marsden, Patrick & Shkoller [11] (hereafter MPS) based on a Lagrangian formulation of the Cartan form.

We take the above leapfrog discretization of (3.3) as an example and, for simplicity, restrict to $\varepsilon = -1$. Then the wave equation (3.3) can be derived from a variational principle using the Lagrangian density

$$\mathcal{L} = L(\partial_t u, \partial_x u, u)\, dx \wedge dt \tag{3.20}$$

with Lagrangian function

$$L(\partial_t u, \partial_x u, u) = \tfrac{1}{2}\,(\partial_t u)^2 - \tfrac{1}{2}\,(\partial_x u)^2 - V(u). \tag{3.21}$$

The wave equation (3.3) is then recoved as the Euler-Lagrange equation

$$\partial_t D_1 L(\partial_t u, \partial_x u, u) + \partial_x D_2 L(\partial_t u, \partial_x u, u) - D_3 L(\partial_t u, \partial_x u, u) = 0 \tag{3.22}$$

where $D_i L$ stands for the partial derivative of L with respect to its ith argument.

The idea of discrete Lagrangian mechanics is to replace the partial derivatives in L by discrete approximations. For example, using a three point approximation over the triangle

$$\triangle_{0,0} = [(0,0), (0,\Delta t), (\Delta x, 0)],$$

one can formulate the discrete Lagrangian density

$$\tilde{L}(u_{1,0}, u_{0,1}, u_{0,0}) = \frac{(u_{0,1} - u_{0,0})^2}{2\Delta t^2} - \frac{(u_{1,0} - u_{0,0})^2}{2\Delta x^2} - V(u_{0,0}) \tag{3.23}$$

where $u_{i,j} = u(i\Delta x, j\Delta t)$, with a corresponding formula for each triangle in (x,t) space.

The associated discrete variational principle provides the following discrete version of the Euler-Lagrange formula at the grid point $(x,t) = (0,0)$

$$D_1\tilde{L}(u_{0,0}, u_{-1,1}, u_{-1,0}) + D_2\tilde{L}(u_{1,-1}, u_{0,0}, u_{0,-1}) + D_3\tilde{L}(u_{1,0}, u_{0,1}, u_{0,0}) = 0 \tag{3.24}$$

which gives rise to the leapfrog discretization

$$\frac{u_{0,1} - 2u_{0,0} + u_{0,-1}}{\Delta t^2} - \frac{u_{1,0} - 2u_{0,0} + u_{-1,0}}{\Delta x^2} = -V'(u_{0,0})\,. \tag{3.25}$$

Therefore, in configuration space, this scheme is equivalent to the staggered leapfrog in (3.18).

We now compare the concept of multi-symplecticity in this Lagrangian setting as proposed by MPS with the concept of multi-symplecticity in the Hamiltonian setting proposed here.

The discrete Lagrangian generates three one forms for the triangle $\triangle_{0,0}$, namely

$$\Theta^1_{0,0} = D_1\tilde{L}(u_{1,0}, u_{0,1}, u_{0,0})d_{1,0} = -\frac{u_{1,0} - u_{0,0}}{\Delta x^2} du_{1,0}, \tag{3.26}$$

$$\Theta^2_{0,0} = D_2\tilde{L}(u_{1,0}, u_{0,1}, u_{0,0})d_{0,1} = \frac{u_{0,1} - u_{0,0}}{\Delta t^2} du_{0,1}, \tag{3.27}$$

and

$$\Theta^3_{0,0} = D_3\tilde{L}(u_{1,0}, u_{0,1}, u_{0,0})d_{0,0} = \frac{u_{0,0} - u_{0,1}}{\Delta t^2} du_{0,0} - \frac{u_{0,0} - u_{1,0}}{\Delta x^2} du_{0,0} - V'(u_{0,0}) du_{0,0}. \tag{3.28}$$

Henceforth, we identify any quantity associated with the triangle

$$\triangle_{i,j} = [((i+1)\Delta x, j\Delta t), (i\Delta x, (j+1)\Delta t), (i\Delta x, j\Delta t)] \tag{3.29}$$

by a subscript (i,j).

If L does not depend explicitly on (t,x), it follows that

$$d\tilde{L}_{i,j} = \Theta^1_{i,j} + \Theta^2_{i,j} + \Theta^3_{i,j} \tag{3.30}$$

and therefore we can conclude that

$$d^2\tilde{L}_{i,j} = 0 = d\Theta^1_{i,j} + d\Theta^2_{i,j} + d\Theta^3_{i,j}. \tag{3.31}$$

for the associated two forms $d\Theta^l_{i,j}$, $l = 1,2,3$.

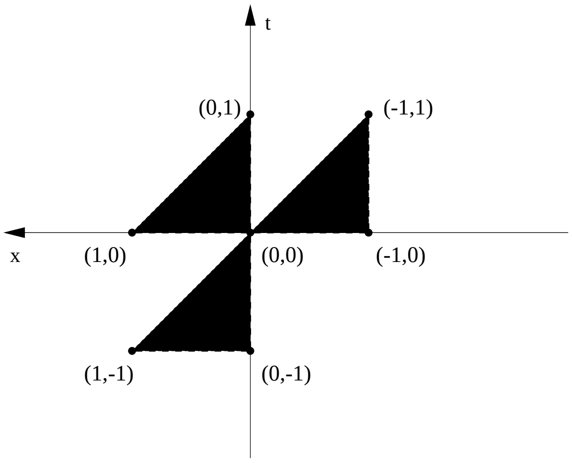

Figure 3: Template for triangular leapfrog scheme of MPS

For the leapfrog discretization, these forms can be calculated explicitly; in particular

$$d\Theta^1_{i,j} = -\frac{1}{\Delta x^2} du_{i+1,j} \wedge du_{i,j}, \tag{3.32}$$

$$d\Theta^2_{i,j} = \frac{1}{\Delta t^2} du_{i,j+1} \wedge du_{i,j}, \tag{3.33}$$

and

$$d\Theta^3_{i,j} = \frac{1}{\Delta x^2} du_{i+1,j} \wedge du_{i,j} - \frac{1}{\Delta t^2} du_{i,j+1} \wedge du_{i,j}. \tag{3.34}$$

These expressions can be used to interpret formula (5.6) in MPS over the domain

$$\mathcal{U} = \triangle_{0,0} \cup \triangle_{0,-1} \cup \triangle_{-1,0}.$$

The region $\mathcal{U}$ has one interior grid point, namely $(0,0)$, and all other grid points in $\mathcal{U}$ are boundary points. Applying now formula (5.6) in MPS leads to

$$\begin{aligned} 0 &= d\Theta^1_{0,0} + d\Theta^2_{0,0} + d\Theta^2_{-1,0} + d\Theta^3_{-1,0} + d\Theta^1_{0,-1} + d\Theta^3_{0,-1} \\ &= d\Theta^1_{0,0} + d\Theta^2_{0,0} - d\Theta^1_{-1,0} - d\Theta^2_{0,-1} \\ &= -\frac{1}{\Delta x^2} du_{1,0} \wedge du_{0,0} + \frac{1}{\Delta t^2} du_{0,1} \wedge du_{0,0} + \frac{1}{\Delta x^2} du_{0,0} \wedge du_{-1,0} - \frac{1}{\Delta t^2} du_{0,0} \wedge du_{0,-1} \end{aligned} \tag{3.35}$$

or, in other words,

$$0 = \frac{du_{0,1} \wedge du_{0,0} - du_{0,0} \wedge du_{0,-1}}{\Delta t^2} - \frac{du_{1,0} \wedge du_{0,0} - du_{0,0} \wedge du_{-1,0}}{\Delta x^2}. \tag{3.36}$$

This expression is a Lagrangian form of conservation of symplecticity. Upon introducing shifted momenta $v_{0,\frac{1}{2}} = (u_{0,1} - u_{0,0})/\Delta t$ and $w_{\frac{1}{2},0} = (u_{1,0} - u_{0,0})/\Delta x$, this scheme is multi-symplectic in the sense of the definition introduced in §2. However, it is not clear that the correspondence between discretizations in the Lagrangrian setting and the definition in §2 will hold in general, particularly for systems with degenerate Lagrangian – such as KdV, KP and water waves – where the Hamiltonian setting is clear.

The leapfrog scheme for nonlinear wave equations – and its analogue for elliptic equations – is one of the simplest and most appealing schemes for numerical integration. However, the multi-symplectic construction involved identifying "momenta" in the x and t directions. Moreover, it is not clear that the energy and momentum conservation properties are as good as other potential schemes (cf. [18]). Indeed, it is known that the symplectic Störmer-Verlet/leapfrog scheme for Hamiltonian ODEs does not conserve any quadratic integrals, even when the system is linear. For Hamiltonian PDEs there is also the question of local versus global preservation of conservation laws (see §§5-6). In the next section we propose an alternative abstract approach to developing multi-symplectic schemes. Rather than consider particular PDEs, we will take as starting point the abstract form of Hamiltonian PDEs proposed in §2, and develop schemes for this class of PDEs, and consider general aspects of their energy and momentum conservation.

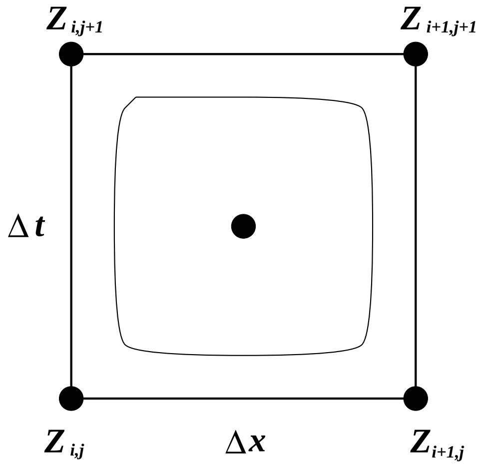

Figure 4: Template for the box scheme

4 Concatenating the midpoint rule: a multi-symplectic box scheme

The midpoint rule is the simplest implicit discretization that leads to a symplectic scheme for Hamiltonian ODEs, and it is the lowest-order scheme in the Gauss-Legendre class of discretizations (cf. [17]). In this section, we concatenate a pair of midpoint discretizations, one in the $t-$direction and one in the $x-$direction. This leads to a box scheme, which we show is multi-symplectic. When the PDE is hyperbolic, the scheme is equivalent to the Preissman box scheme, which was introduced by Preissman in 1960 and is one of the most widely used schemes in hydraulics (cf. [1],[2]).

However, we make no assumption about the type – elliptic, hyperbolic, etc. – about the partial differentical equation. We assume only that the PDE can be written in the abstract general form (2.1). In addition to its symplectic conservation property, we show that this scheme has excellent discrete energy and momentum conservation properties. We also show that the multi-symplectic conservation property is not robust to changes in discretiztion. For example, we show that the box scheme is *not* multi-symplectic when the centroid of the discretization is perturbed away from the box centre.

Introduce a uniform grid (x_i, t_j) in $\mathbb{R}^2$ with mesh-length Δt in the $t-$direction and mesh-length Δx in the $x-$direction. The value of $\boldsymbol{z}(x,t)$ at the mesh point (x_i, t_j) is denoted by $\boldsymbol{z}_{i,j}$. The layout of a typical box is shown in Figure 4.

We start by discretizing (2.1) in time by the implicit midpoint rule. This yields the semi-discretization

$$\frac{d}{dx}\mathbf{K}\boldsymbol{z}_{j+\frac{1}{2}} = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}_{j+\frac{1}{2}}) - \mathbf{M}\frac{\boldsymbol{z}_{j+1} - \boldsymbol{z}_j}{\Delta t}\,, \tag{4.1}$$

with corresponding semi-discretized multi-symplectic structure

$$\frac{d}{dx}\boldsymbol{\kappa}(U_{j+\frac{1}{2}}, V_{j+\frac{1}{2}}) + \frac{\boldsymbol{\omega}(U_{j+1}, V_{j+1}) - \boldsymbol{\omega}(U_j, V_j)}{\Delta t} = 0\,, \tag{4.2}$$

where U_j, V_j are any two solutions of the semi-discretization of the variational equation.

For the discretization in the x-direction, we apply the implicit midpoint rule again. Concatenating the two midpoint rules leads to the following discrete version of (2.1)

$$\mathbf{M}\left(\frac{\boldsymbol{z}_{i+\frac{1}{2},j+1} - \boldsymbol{z}_{i+\frac{1}{2},j}}{\Delta t}\right) + \mathbf{K}\left(\frac{\boldsymbol{z}_{i+1,j+\frac{1}{2}} - \boldsymbol{z}_{i,j+\frac{1}{2}}}{\Delta x}\right) = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}_{i+\frac{1}{2},j+\frac{1}{2}})\,, \tag{4.3}$$

where

$$\boldsymbol{z}_{i+\frac{1}{2},j} = \tfrac{1}{2}(\boldsymbol{z}_{i,j} + \boldsymbol{z}_{i+1,j})\,, \quad \boldsymbol{z}_{i,j+\frac{1}{2}} = \tfrac{1}{2}(\boldsymbol{z}_{i,j} + \boldsymbol{z}_{i,j+1}) \tag{4.4}$$

and

$$\boldsymbol{z}_{i+\frac{1}{2},j+\frac{1}{2}} = \tfrac{1}{4}(\boldsymbol{z}_{i,j} + \boldsymbol{z}_{i+1,j} + \boldsymbol{z}_{i,j+1} + \boldsymbol{z}_{i+1,j+1})\,. \tag{4.5}$$

We call this scheme *the centred box scheme.*

Theorem. *The centred box discretization (4.3) is multi-symplectic: in each box the discretization satisfies*

$$\frac{\boldsymbol{\omega}_{i+\frac{1}{2},j+1}-\boldsymbol{\omega}_{i+\frac{1}{2},j}}{\Delta t}+\frac{\boldsymbol{\kappa}_{i+1,j+\frac{1}{2}}-\boldsymbol{\kappa}_{i,j+\frac{1}{2}}}{\Delta x}=0 \tag{4.6}$$

where

$$\boldsymbol{\omega}_{i,j}=\langle \mathbf{M}U_{i,j},V_{i,j}\rangle \quad\text{and}\quad \boldsymbol{\kappa}_{i,j}=\langle \mathbf{K}U_{i,j},V_{i,j}\rangle\,, \tag{4.7}$$

and $\{U_{i,j}\}$ and $\{V_{i,j}\}$ are any two solutions of the discrete variational equation associated with (4.3).

To prove this result, we first introduce the discrete variational equation associated with (4.3)

$$\mathbf{M}\left(\frac{\boldsymbol{dz}_{i+\frac{1}{2},j+1}-\boldsymbol{dz}_{i+\frac{1}{2},j}}{\Delta t}\right)+\mathbf{K}\left(\frac{\boldsymbol{dz}_{i+1,j+\frac{1}{2}}-\boldsymbol{dz}_{i,j+\frac{1}{2}}}{\Delta x}\right)=\boldsymbol{A}_{i+\frac{1}{2},j+\frac{1}{2}}\boldsymbol{dz}_{i+\frac{1}{2},j+\frac{1}{2}}\,, \tag{4.8}$$

where

$$\boldsymbol{A}_{i+\frac{1}{2},j+\frac{1}{2}}=\boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z}_{i+\frac{1}{2},j+\frac{1}{2}})\,.$$

Let $U_{i,j}$ and $V_{i,j}$ be any two solutions of (4.8). Take the inner product of $U_{i+\frac{1}{2},j+\frac{1}{2}}$ with (4.8) evaluated at $V_{i,j}$, and take the inner product of $V_{i+\frac{1}{2},j+\frac{1}{2}}$ with (4.8) evaluated at $U_{i,j}$. Subtracting these two equations leads to

$$\begin{aligned}\mathcal{F}(U_{i,j},V_{i,j}) &= \langle V_{i+\frac{1}{2},j+\frac{1}{2}},\boldsymbol{A}_{i+\frac{1}{2},j+\frac{1}{2}}U_{i+\frac{1}{2},j+\frac{1}{2}}\rangle-\langle U_{i+\frac{1}{2},j+\frac{1}{2}},\boldsymbol{A}_{i+\frac{1}{2},j+\frac{1}{2}}V_{i+\frac{1}{2},j+\frac{1}{2}}\rangle\\ &= \frac{1}{\Delta t}\boldsymbol{\omega}(U_{i+\frac{1}{2},j+1}-U_{i+\frac{1}{2},j},V_{i+\frac{1}{2},j+\frac{1}{2}})-\frac{1}{\Delta t}\boldsymbol{\omega}(V_{i+\frac{1}{2},j+1}-V_{i+\frac{1}{2},j},U_{i+\frac{1}{2},j+\frac{1}{2}})\\ &\quad+\frac{1}{\Delta x}\boldsymbol{\kappa}(U_{i+1,j+\frac{1}{2}}-U_{i,j+\frac{1}{2}},V_{i+\frac{1}{2},j+\frac{1}{2}})-\frac{1}{\Delta x}\boldsymbol{\kappa}(V_{i+1,j+\frac{1}{2}}-V_{i,j+\frac{1}{2}},U_{i+\frac{1}{2},j+\frac{1}{2}})\,.\end{aligned}$$

Now, using the fact that

$$\boldsymbol{z}_{i+\frac{1}{2},j+\frac{1}{2}}=\tfrac{1}{2}(\boldsymbol{z}_{i+\frac{1}{2},j+1}+\boldsymbol{z}_{i+\frac{1}{2},j})=\tfrac{1}{2}(\boldsymbol{z}_{i+1,j+\frac{1}{2}}+\boldsymbol{z}_{i,j+\frac{1}{2}})\,,$$

we find

$$\boldsymbol{\omega}(U_{i+\frac{1}{2},j+1}-U_{i+\frac{1}{2},j},V_{i+\frac{1}{2},j+\frac{1}{2}})-\boldsymbol{\omega}(V_{i+\frac{1}{2},j+1}-V_{i+\frac{1}{2},j},U_{i+\frac{1}{2},j+\frac{1}{2}})=\delta\boldsymbol{\omega}_{i,j}\,, \tag{4.9}$$

where

$$\delta\boldsymbol{\omega}_{i,j}=\boldsymbol{\omega}(U_{i+\frac{1}{2},j+1},V_{i+\frac{1}{2},j+1})-\boldsymbol{\omega}(U_{i+\frac{1}{2},j},V_{i+\frac{1}{2},j})=\boldsymbol{\omega}_{i+\frac{1}{2},j}-\boldsymbol{\omega}_{i+\frac{1}{2},j}\,, \tag{4.10}$$

and

$$\boldsymbol{\kappa}(U_{i+1,j+\frac{1}{2}}-U_{i,j+\frac{1}{2}},V_{i+\frac{1}{2},j+\frac{1}{2}})-\boldsymbol{\kappa}(V_{i+1,j+\frac{1}{2}}-V_{i,j+\frac{1}{2}},U_{i+\frac{1}{2},j+\frac{1}{2}})=\delta\boldsymbol{\kappa}_{i,j}\,, \tag{4.11}$$

where

$$\delta\boldsymbol{\kappa}_{i,j}=\boldsymbol{\kappa}(U_{i+1,j+\frac{1}{2}},V_{i+1,j+\frac{1}{2}})-\boldsymbol{\kappa}(U_{i,j+\frac{1}{2}},V_{i,j+\frac{1}{2}})=\boldsymbol{\kappa}_{i+1,j+\frac{1}{2}}-\boldsymbol{\kappa}_{i,j+\frac{1}{2}}\,. \tag{4.12}$$

Combining (4.9) and (4.11) leads to

$$\frac{\boldsymbol{\omega}_{i+\frac{1}{2},j+1}-\boldsymbol{\omega}_{i+\frac{1}{2},j}}{\Delta t}+\frac{\boldsymbol{\kappa}_{i+1,j+\frac{1}{2}}-\boldsymbol{\kappa}_{i,j+\frac{1}{2}}}{\Delta x}=\langle V_{i+\frac{1}{2},j+\frac{1}{2}},\left(\boldsymbol{A}_{i+\frac{1}{2},j+\frac{1}{2}}-\boldsymbol{A}^T_{i+\frac{1}{2},j+\frac{1}{2}}\right)U_{i+\frac{1}{2},j+\frac{1}{2}}\rangle\,, \tag{4.13}$$

and the result (4.6) now follows from the symmetry of $\boldsymbol{A}_{i+\frac{1}{2},j+\frac{1}{2}}$.

It is also clear from (4.13) that the multi-symplectic property of the discretization (4.3) depends crucially on the centering of the term $\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z}_{i+\frac{1}{2},j+\frac{1}{2}})$ in (4.3). For example, suppose the term $\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z})$ is off-centred slightly; let

$$\begin{aligned}\tilde{\boldsymbol{z}}_{i,j} &= (\tfrac{1}{2}+\varepsilon)\boldsymbol{z}_{i,j+\frac{1}{2}}+(\tfrac{1}{2}-\varepsilon)\boldsymbol{z}_{i+1,j+\frac{1}{2}}\\ &= \boldsymbol{z}_{i+\frac{1}{2},j+\frac{1}{2}}+\varepsilon(\boldsymbol{z}_{i,j+\frac{1}{2}}-\boldsymbol{z}_{i+1,j+\frac{1}{2}})\,,\end{aligned}$$

and replace the right-hand side of (4.3) with $\boldsymbol{\nabla}_{\boldsymbol{z}}S(\tilde{\boldsymbol{z}}_{i,j})$ Then repeating the above analysis leads to the following $\varepsilon-$modification of (4.13)

$$\frac{\boldsymbol{\omega}_{i+\frac{1}{2},j+1}-\boldsymbol{\omega}_{i+\frac{1}{2},j}}{\Delta t}+\frac{\boldsymbol{\kappa}_{i+1,j+\frac{1}{2}}-\boldsymbol{\kappa}_{i,j+\frac{1}{2}}}{\Delta x}=\varepsilon\langle U_{i,j+\frac{1}{2}},\tilde{\boldsymbol{A}}_{i,j}V_{i+\frac{1}{2},j+\frac{1}{2}}\rangle-\varepsilon\langle V_{i,j+\frac{1}{2}},\tilde{\boldsymbol{A}}_{i,j}U_{i+\frac{1}{2},j+\frac{1}{2}}\rangle\,, \tag{4.14}$$

where

$$\tilde{\boldsymbol{A}}_{i,j} = \boldsymbol{D}_{\boldsymbol{z}\boldsymbol{z}} S(\tilde{z}_{i,j})\,.$$

The right-hand side of (4.14) does not vanish in general: off-centering the $\boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z})$ term leads to a numerical discretization which is *not* multi-symplectic.

In the next section we consider the energy and momentum conservation properties of this multi-symplectic box scheme.

5 Local energy and momentum conservation

For Hamiltonian ODEs which do not depend explicitly on time, level sets of the Hamiltonian function – or energy – are preserved:

$$\mathbf{J}\boldsymbol{z}_t = \boldsymbol{\nabla}_{\boldsymbol{z}} H(\boldsymbol{z})\,, \quad \boldsymbol{z} \in \mathbb{R}^{2n} \quad \Rightarrow \quad \frac{d}{dt} H(\boldsymbol{z}) = 0\,.$$

For multi-symplectic PDEs of the form (2.1), when $S(Z)$ does not depend explicitly on space or time there are two conservation laws. *Conservation of energy* is associated with the translation invariance in time and *conservation of momentum* is associated with the translation invariance in space.

In contrast to Hamiltonian ODEs, the Hamiltonian function $S(\boldsymbol{z})$ associated with the multi-symplectic system (2.1) will not be conserved in any sense; a straightforward calculation shows that

$$\begin{aligned}
\frac{\partial}{\partial t} S(\boldsymbol{z}) &= \langle \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}), \boldsymbol{z}_t \rangle = \langle \mathbf{K}\boldsymbol{z}_x, \boldsymbol{z}_t \rangle = \boldsymbol{\kappa}(\boldsymbol{z}_x, \boldsymbol{z}_t) && (5.1)\\
\frac{\partial}{\partial x} S(\boldsymbol{z}) &= \langle \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}), \boldsymbol{z}_x \rangle = \langle \mathbf{M}\boldsymbol{z}_t, \boldsymbol{z}_x \rangle = \boldsymbol{\omega}(\boldsymbol{z}_t, \boldsymbol{z}_x)\,. && (5.2)
\end{aligned}$$

However, the conservation laws for energy and momentum can be completely characterized in terms of $S(\boldsymbol{z})$, $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}$. For any system of the form (2.1), conservation of energy and momentum take the following form respectively

$$\partial_t E(\boldsymbol{z}) + \partial_x F(\boldsymbol{z}) = 0 \quad \text{and} \quad \partial_t I(\boldsymbol{z}) + \partial_x G(\boldsymbol{z}) = 0\,,$$

where E, F, I and G are defined in (1.34) (cf. [5]).

It is well known that *linear* Hamiltonian ODEs with Gauss-Legendre symplectic discretizations conserve energy exactly (indeed, any quadratic invariant) (cf. [17]). Therefore it is natural to enquire whether the concatenation of the mid-point rule introduced in §4 will preserve the energy conservation law or other conservation laws. In this section we prove the remarkable result that abstract linear Hamiltonian PDEs in multi-symplectic form – discretized with the centred box scheme – conserve energy *and* momentum exactly; moreover, it is the *local* energy and momentum conservation that is preserved by the discretization. This local conservation property is stronger than global conservation (see §6 for discussion of global energy and momentum conservation).

Theorem. *When $S(\boldsymbol{z})$ is quadratic in $\boldsymbol{z}$, the multi-symplectic box scheme (4.3) conserves discrete energy and momentum exactly.*

To prove this Theorem, we need the following preliminary result.

Proposition. *Let $S(\boldsymbol{z}) = \frac{1}{2}\langle \boldsymbol{z}, \mathbf{A}\boldsymbol{z}\rangle$ and suppose $\boldsymbol{z}_{i,j}$ satisfies (4.3). Then*

$$\begin{aligned}
S(\boldsymbol{z}_{i+\frac{1}{2},j+1}) - S(\boldsymbol{z}_{i+\frac{1}{2},j}) &= \frac{1}{\Delta x}\boldsymbol{\kappa}(\boldsymbol{z}_{i+1,j+\frac{1}{2}} - \boldsymbol{z}_{i,j+\frac{1}{2}}, \boldsymbol{z}_{i+\frac{1}{2},j+1} - \boldsymbol{z}_{i+\frac{1}{2},j}) && (5.3)\\
S(\boldsymbol{z}_{i+1,j+\frac{1}{2}}) - S(\boldsymbol{z}_{i,j+\frac{1}{2}}) &= \frac{1}{\Delta t}\boldsymbol{\omega}(\boldsymbol{z}_{i+\frac{1}{2},j+1} - \boldsymbol{z}_{i+\frac{1}{2},j}, \boldsymbol{z}_{i+1,j+\frac{1}{2}} - \boldsymbol{z}_{i,j+\frac{1}{2}}) && (5.4)
\end{aligned}$$

These two equations are discrete analogues of (5.1)-(5.2). The first identity is proved by taking the inner product of (4.3) with $(\boldsymbol{z}_{i+\frac{1}{2},j+1} - \boldsymbol{z}_{i+\frac{1}{2},j})/\Delta t$ and using the skew-symmetry of $\mathbf{M}$. Similarly, the second identity is proved by taking the inner product of (4.3) with $(\boldsymbol{z}_{i+1,j+\frac{1}{2}} - \boldsymbol{z}_{i,j+\frac{1}{2}})/\Delta x$ and using the skew symmetry of $\mathbf{K}$.

Discrete conservation of energy is then established as follows. A straightforward substitution using the definitions of $E_{i,j}$ and $F_{i,j}$ leads to

$$\frac{E_{i+\frac{1}{2},j+1}-E_{i+\frac{1}{2},j}}{\Delta t}+\frac{F_{i+1,j+\frac{1}{2}}-F_{i,j+\frac{1}{2}}}{\Delta x}=\frac{1}{2\Delta t\Delta x}\{\mathcal{K}_{i,j}\}\,, \tag{5.5}$$

where

$$\begin{aligned}\mathcal{K}_{i,j} \;=\;& \boldsymbol{\kappa}(\boldsymbol{z}_{i+1,j+\frac{1}{2}}-\boldsymbol{z}_{i,j+\frac{1}{2}},\boldsymbol{z}_{i+\frac{1}{2},j+1}-\boldsymbol{z}_{i+\frac{1}{2},j})\\ &-\tfrac{1}{2}\boldsymbol{\kappa}(\boldsymbol{z}_{i+1,j+1}-\boldsymbol{z}_{i,j+1},\boldsymbol{z}_{i+\frac{1}{2},j+1})+\tfrac{1}{2}\boldsymbol{\kappa}(\boldsymbol{z}_{i+1,j}-\boldsymbol{z}_{i,j},\boldsymbol{z}_{i+\frac{1}{2},j})\\ &+\tfrac{1}{2}\boldsymbol{\kappa}(\boldsymbol{z}_{i+1,j+1}-\boldsymbol{z}_{i+1,j},\boldsymbol{z}_{i+1,j+\frac{1}{2}})-\tfrac{1}{2}\boldsymbol{\kappa}(\boldsymbol{z}_{i,j+1}-\boldsymbol{z}_{i,j},\boldsymbol{z}_{i,j+\frac{1}{2}})\}\end{aligned} \tag{5.6}$$

using the definitions (1.34), the Proposition and the identities

$$F_{i+1,j+\frac{1}{2}}=\frac{1}{2\Delta t}\boldsymbol{\kappa}(\boldsymbol{z}_{i+1,j+1}-\boldsymbol{z}_{i+1,j},\boldsymbol{z}_{i+1,j+\frac{1}{2}})\quad\text{and}\quad F_{i,j+\frac{1}{2}}=\frac{1}{2\Delta t}\boldsymbol{\kappa}(\boldsymbol{z}_{i,j+1}-\boldsymbol{z}_{i,j},\boldsymbol{z}_{i,j+\frac{1}{2}})\,.$$

By expanding each of the terms in $\mathcal{K}_{i,j}$ and using the skew-symmetry of $\boldsymbol{\kappa}$, we find that $\mathcal{K}_{i,j}$ vanishes identically, proving discrete conservation of energy.

A similar argument is used to prove discrete conservation of momentum; by the definition of $I(\boldsymbol{z})$ and $G(\boldsymbol{z})$,

$$\frac{I_{i+\frac{1}{2},j+1}-I_{i+\frac{1}{2},j}}{\Delta t}+\frac{G_{i+1,j+\frac{1}{2}}-G_{i,j+\frac{1}{2}}}{\Delta x}=\frac{1}{2\Delta t\Delta x}\{\mathcal{M}_{i,j}\}\,, \tag{5.7}$$

where

$$\begin{aligned}\mathcal{M}_{i,j} \;=\;& \boldsymbol{\omega}(\boldsymbol{z}_{i+\frac{1}{2},j+1}-\boldsymbol{z}_{i+\frac{1}{2},j},\boldsymbol{z}_{i+1,j+\frac{1}{2}}-\boldsymbol{z}_{i,j+\frac{1}{2}})\\ &+\tfrac{1}{2}\boldsymbol{\omega}(\boldsymbol{z}_{i+1,j+1}-\boldsymbol{z}_{i,j+1},\boldsymbol{z}_{i+\frac{1}{2},j+1})-\tfrac{1}{2}\boldsymbol{\omega}(\boldsymbol{z}_{i+1,j}-\boldsymbol{z}_{i,j},\boldsymbol{z}_{i+\frac{1}{2},j})\\ &-\tfrac{1}{2}\boldsymbol{\omega}(\boldsymbol{z}_{i+1,j+1}-\boldsymbol{z}_{i+1,j},\boldsymbol{z}_{i+1,j+\frac{1}{2}})+\tfrac{1}{2}\boldsymbol{\omega}(\boldsymbol{z}_{i,j+1}-\boldsymbol{z}_{i,j},\boldsymbol{z}_{i,j+\frac{1}{2}})\}\end{aligned} \tag{5.8}$$

using the definitions (1.34), the Proposition and the identities

$$I_{i+\frac{1}{2},j+1}=\frac{1}{2\Delta x}\boldsymbol{\omega}(\boldsymbol{z}_{i+1,j+1}-\boldsymbol{z}_{i,j+1},\boldsymbol{z}_{i+\frac{1}{2},j+1})\quad\text{and}\quad I_{i+\frac{1}{2},j}=\frac{1}{2\Delta x}\boldsymbol{\omega}(\boldsymbol{z}_{i+1,j}-\boldsymbol{z}_{i,j},\boldsymbol{z}_{i+\frac{1}{2},j})\,.$$

By expanding each of the terms in $\mathcal{M}$ and using the skew-symmetry of $\boldsymbol{\omega}$ we find that it vanishes identically, proving discrete conservation of momentum. This completes the proof of the Theorem.

One of the remarkable features of this result is that the energy, momentum, and the fluxes are not algebraic functions – they depend on derivatives. But, with the box scheme these derivatives are all aligned in a natural way so that the discrete conservation of energy and momentum are exact.

Numerical experiments show that conservation of energy and momentum for the multi-symplectic box scheme are also excellent when the system is *nonlinear* (cf. Reich [16]).

6 Global properties of multi-symplectic numerical schemes

Discrete conservation of symplecticity, discrete conservation of energy and discrete conservation of momentum are all *local* properties of a numerical scheme. Locality is the natural setting for discretizations such as finite difference discretizations. On the other hand, a natural question is what global properties a numerical scheme has; that is, what properties the coupled system has when summed (discrete integration) over all spatial grid points. We don't consider this question in detail, but use this section to show how a local property leads naturally to a global property. Boundary conditions are crucial here, because boundary conditions may or may not respect a conservation law. For example, the wave equation

$$u_{tt}-u_{xx}+V'(u)=0\,,\quad\text{with}\quad 0<x<L\,, \tag{6.1}$$

and natural boundary conditions

$$u_x(0,t) = 0 \quad \text{and} \quad u_t(L,t) + \nu u_x(L,t) = 0\,, \tag{6.2}$$

with ν some nonzero real number, is *not* globally-symplectic and does not conserve global-energy (i.e. when these quantities are integrated over x). For example

$$\frac{d}{dt}\int_0^L [\tfrac{1}{2}u_t^2 + \tfrac{1}{2}u_x^2 + V(u)]\,dx = -\nu u_x^2|_{x=L}\,, \tag{6.3}$$

and

$$\frac{d}{dt}\int_0^L \boldsymbol{d}u \wedge \boldsymbol{d}u_t\,dx = -\nu^{-1}\,\boldsymbol{d}u \wedge \boldsymbol{d}u_t|_{x=L}\,. \tag{6.4}$$

On the other hand, away from the boundaries, the continuous system or the discretization (using the box scheme for example) applied to this wave equation conserves symplecticity locally and it conserves energy locally (when $V(u)$ is quadratic).

However, we will show that if the boundary conditions respect the structure (symplecticity, energy, momentum), then discrete local conservation implies discrete global conservation.

For example, we consider a class of wave equations with periodic boundary conditions $u(x=0,t) = u(x=L,t)$ etc. In this case, the multi-symplectic box scheme from §4, for example, gives rise to the identity

$$\sum_{i=0}^{N-1}\left[\boldsymbol{\kappa}_{i+1,j+\frac{1}{2}} - \boldsymbol{\kappa}_{i,j+\frac{1}{2}}\right] = \boldsymbol{\kappa}_{N,j+\frac{1}{2}} - \boldsymbol{\kappa}_{0,j+\frac{1}{2}} = 0 \tag{6.5}$$

where the summation is over all grid points in the spatial direction. Here we have used the property that periodicity of the problem implies $\boldsymbol{\kappa}_{0,j+\frac{1}{2}} = \boldsymbol{\kappa}_{N,j+\frac{1}{2}}$ for all j. This and the discrete conservation of multi-symplecticity (4.6) result in

$$\frac{1}{\Delta t}\left(\sum_{i=0}^{N-1}\boldsymbol{\omega}_{i+\frac{1}{2},j+1} - \sum_{i=0}^{N}\boldsymbol{\omega}_{i+\frac{1}{2},j}\right)\Delta x = 0\,. \tag{6.6}$$

This result implies the conservation of the "standard" wedge product under a symplectic time discretization, i.e., upon introducing

$$\overline{\boldsymbol{\omega}}_j = \sum_{i=0}^{N-1}\boldsymbol{\omega}_{i+\frac{1}{2},j}\Delta x\,, \tag{6.7}$$

we obtain

$$\overline{\boldsymbol{\omega}}_{j+1} = \overline{\boldsymbol{\omega}}_j. \tag{6.8}$$

Note that (6.5) is a discretization of

$$\int_{x=0}^{L}\left[\frac{\partial}{\partial x}\boldsymbol{\kappa}\right]dx = \boldsymbol{\kappa}(x=L,t) - \boldsymbol{\kappa}(x=0,t) = 0 \tag{6.9}$$

and that (6.6) is a discretization of

$$\int_{x=0}^{L}\left[\frac{\partial}{\partial t}\boldsymbol{\omega}\right]dx = \frac{\partial}{\partial t}\left[\int_{x=0}^{L}\boldsymbol{\omega}\,dx\right] = \frac{d}{dt}\overline{\boldsymbol{\omega}} = 0 \tag{6.10}$$

In fact, one could first discretize the wave equation (6.1) in the spatial direction to obtain a finite dimensional Hamiltonian ODE which is then discretized in time by a symplectic method. This approach is explained in more detail in [14]. The disadvantage of such an approach is that one has to treat the x- and t-directions in a particular order and that the formulation is not local (i.e. requires the consideration of boundary conditions and is symplectic only after summing over all spatial grid point) unlike the multi-symplectic formulation.

Another interesting conserved quantity is related to the integral of (1.22) over a rectangular domain $\mathcal{D} = [0, L] \times [0, T]$ which yields the identity

$$
\begin{aligned}
0 &= \int_{x=0}^{L} \int_{t=0}^{T} \left(\frac{\partial}{\partial t} \boldsymbol{\omega} + \frac{\partial}{\partial x} \boldsymbol{\kappa} \right) dx dt \\
&= \int_{x=0}^{L} \left(\boldsymbol{\omega}|_{t=T} - \boldsymbol{\omega}|_{t=0} \right) dx + \int_{t=0}^{T} \left(\boldsymbol{\kappa}|_{x=L} - \boldsymbol{\kappa}|_{x=0} \right) dt.
\end{aligned}
$$

Upon taking $\mathcal{D} = [x_0, x_N] \times [t_0, t_M]$, we obtain the following discrete version using (4.6):

$$
\begin{aligned}
0 &= \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \left(\frac{\boldsymbol{\omega}_{i+\frac{1}{2},j+1} - \boldsymbol{\omega}_{i+\frac{1}{2},j}}{\Delta t} + \frac{\boldsymbol{\kappa}_{i+1,j+\frac{1}{2}} - \boldsymbol{\kappa}_{i,j+\frac{1}{2}}}{\Delta x} \right) \Delta x \Delta t \\
&= \sum_{i=0}^{N-1} \left(\boldsymbol{\omega}_{i+\frac{1}{2},M} - \boldsymbol{\omega}_{i+\frac{1}{2},0} \right) \Delta x + \sum_{j=0}^{M-1} \left(\boldsymbol{\kappa}_{N,j+\frac{1}{2}} - \boldsymbol{\kappa}_{0,j+\frac{1}{2}} \right) \Delta t.
\end{aligned}
$$

7 Concluding Remarks

In this paper we have introduced the concept of *discrete conservation of symplecticity* for discretizations of Hamiltonian PDEs. This property is local, and we showed that – for a centred box discretization – it also leads to exact discrete conservation of energy and momentum for linear Hamiltonian PDEs. This local property is stronger than the global property that summation over all spatial grid points leads to a discrete symplectic scheme in the time direction: indeed we have shown that – with compatible boundary conditions – the local property implies the global property. On the other hand, if the boundary conditions are not compatible with the symplectic structure, it is still possible for the scheme to be locally multi-symplectic at every interior cell.

We showed that various well-known methods for the nonlinear wave equation are indeed multi-symplectic which gives another explanation for their superior long time behavior over general purpose methods. We anticipate that the notion of multi-symplectic integration will prove very useful in understanding existing methods and, more importantly, will lead to the development of new schemes with excellent long time stability properties. Indeed, the study of the stability, accuracy and error analysis of such discretizations is an open question. For example do the powerful techniques of backward error analysis extend to symplectic PDEs?

A separate and interesting question not considered here is the development of numerical methods for solving the coupled system of discrete equations; however the most natural techniques for nonlinear hyperbolic PDEs discretized by a box scheme are the double sweep techniques initiated by Preissman, which have now been considerable improved and extended to more than one space dimensions (cf. [1]).

The concept of a multi-symplectic integrator extends naturally to higher space dimension. A canonical form for Hamiltonian PDEs on K space dimensions is

$$
\mathbf{M} \boldsymbol{z}_t + \sum_{k=1}^{K} \mathbf{K}_k \boldsymbol{z}_{x_k} = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}), \quad \boldsymbol{z} \in \mathbb{R}^m, \quad m \geq 2, \tag{7.1}
$$

where K is the number of independent space directions which will be denoted by x_k, and $\mathbf{M}$, $\mathbf{K}_k$ are skew-symmetric matrices. An example of a system that can be formulated in this way is the generalized KP equation:

$$
\frac{\partial}{\partial x_1} \left(2 \frac{\partial u}{\partial t} + \frac{\partial}{\partial x_1} f(u) + \frac{\partial^3 u}{\partial x_1^3} \right) + \sigma \frac{\partial^2 u}{\partial x_2^2} = 0 \tag{7.2}
$$

where σ is a non-zero parameter, $f(u)$ is some smooth function. It is straightforward to reformulate (7.2) into the form (7.1) with $m = 8$ and $\mathbf{K}_1$ non-degenerate; see Bridges [7] for details. Many other Hamiltonian PDEs can be formulated as in (7.1) including the governing equations for water waves (cf. [5]).

An immediate consequence of the form of the equations (7.1) is the existence of a generalization of conservation of symplecticity:

$$\frac{\partial}{\partial t}\boldsymbol{\omega}(U,V)+\frac{\partial}{\partial x_1}\boldsymbol{\kappa}^{(1)}(U,V)+\frac{\partial}{\partial x_2}\boldsymbol{\kappa}^{(2)}(U,V)=0\,, \tag{7.3}$$

where

$$\boldsymbol{\omega}(U,V)=\langle \mathbf{M}U,V\rangle\,,\quad \boldsymbol{\kappa}^{(1)}(U,V)=\langle \mathbf{K}_1U,V\rangle\,,\quad \boldsymbol{\kappa}^{(2)}(U,V)=\langle \mathbf{K}_2U,V\rangle\,, \tag{7.4}$$

and U and V are any solutions of the variational equation associated with (7.1)

$$\mathbf{M}\boldsymbol{dz}_t+\sum_{k=1}^{K}\mathbf{K}_k\boldsymbol{dz}_{x_k}=\boldsymbol{D}_{\boldsymbol{zz}}S(\boldsymbol{z})\boldsymbol{dz}\,,\quad \boldsymbol{dz}\in\mathbb{R}^m\,. \tag{7.5}$$

A natural generalization of *multi-symplectic integrator* to systems of the form (7.1) is characterized by discretizations that conserve a discrete version of (7.5) similar to (2.7). A natural conjecture is that the multi-symplectic box scheme of §4 extends to a multi-symplectic box scheme for systems of the form (7.1).

A systematic way to obtain multi-symplectic methods is of great interest as well as an understanding of their long-time approximation properties. As suggested in Reich [16], higher order multi-symplectic box schemes could be obtained by using higher order variants of the implicit midpoint method for the discretization of the t- and/or x-directions such as the symplectic Gauss-Legrende methods [17].

For example, let us discretize (2.10) in time by the implicit midpoint rule. This yields the semi-discretization

$$\frac{d}{dx}\mathbf{K}\boldsymbol{z}_{j+\frac12}=\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z}_{j+\frac12})-\mathbf{M}\frac{\boldsymbol{z}_{j+1}-\boldsymbol{z}_j}{\Delta t}\,.$$

For the discretization in the x-direction, we apply the fourth order Gauss-Legrende method [17] and obtain

$$\begin{aligned}\mathbf{K}\frac{\boldsymbol{z}_{i+\frac{k}{3},j+\frac12}-\boldsymbol{z}_{i,j+\frac12}}{\Delta x}&=\sum_{l=1}^{2}a_{kl}\left(\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z}_{i+\frac{l}{3},j+\frac12})-\mathbf{M}\frac{\boldsymbol{z}_{i+\frac{l}{3},j+1}-\boldsymbol{z}_{i+\frac{l}{3},j}}{\Delta t}\right), \qquad k=1,2,\\ \mathbf{K}\frac{\boldsymbol{z}_{i+1,j+\frac12}-\boldsymbol{z}_{i,j+\frac12}}{\Delta x}&=\frac12\sum_{l=1}^{2}\left(\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z}_{i+\frac{l}{3},j+\frac12})-\mathbf{M}\frac{\boldsymbol{z}_{i+\frac{l}{3},j+1}-\boldsymbol{z}_{i+\frac{l}{3},j}}{\Delta t}\right),\end{aligned}$$

with

$$a_{11}=\frac14,\quad a_{12}=\frac14-\frac{\sqrt3}{6},\quad a_{21}=\frac14+\frac{\sqrt3}{6},\quad a_{22}=\frac14.$$

This gives rise to the discrete conservation law

$$0=\frac{\boldsymbol{\omega}_{i+1,j+\frac12}-\boldsymbol{\omega}_{i,j+\frac12}}{\Delta x}+\sum_{l=1}^{2}\frac{\boldsymbol{\kappa}_{i+\frac{l}{3},j+1}-\boldsymbol{\kappa}_{i+\frac{l}{3},j}}{2\Delta t}\,.$$

Essentially, the two-dimensional concatenation of the basic ODE schemes should lead to a higher order approximation at the boundary of the Δx-Δt cell. Furthermore, the concatenation preserves the multi-symplectic structure of the basic method and the overall scheme will be higher-order and multi-symplectic. See Reich [16] for complete details of this generalization.

Another advantage of the local definition of symplecticity is that the implication of non-symplectic terms can be tested. For example, perturbed multi-symplectic systems of the form

$$\mathbf{M}\boldsymbol{z}_t+\mathbf{K}\boldsymbol{z}_x=\boldsymbol{\nabla}_{\boldsymbol{z}}S(\boldsymbol{z})+\varepsilon F(\boldsymbol{z})\,,\quad \boldsymbol{z}\in\mathrm{R}^n\,, \tag{7.6}$$

lead to the following perturbed conservation equation for symplecticity

$$\frac{\partial}{\partial t}\boldsymbol{\omega}+\frac{\partial}{\partial x}\boldsymbol{\kappa}=\varepsilon\langle(\boldsymbol{D}_{\boldsymbol{z}}F(\boldsymbol{z})-\boldsymbol{D}_{\boldsymbol{z}}F(\boldsymbol{z})^T)U,V\rangle\,. \tag{7.7}$$

To see the implications of such perturbations consider the following forced-damped nonlinear wave equation

$$u_{tt}+\varepsilon u_t-u_{xx}+V'(u)=f(x,t)\,, \tag{7.8}$$

where $u(x,t)$ is scalar valued, $\varepsilon > 0$, $V(u)$ is some smooth nonlinear function and $f(x,t)$ is a forcing function. Let

$$\boldsymbol{\omega} = \boldsymbol{d}u \wedge \boldsymbol{d}u_t \quad \text{and} \quad \boldsymbol{\kappa} = \boldsymbol{d}u_x \wedge \boldsymbol{d}u \, .$$

Then a straightforward calculation, using the variational equation associated with (7.8)

$$\boldsymbol{d}u_{tt} + \varepsilon \boldsymbol{d}u_t - \boldsymbol{d}u_{xx} + V''(u)\boldsymbol{d}u = 0 \, ,$$

results in

$$\frac{\partial}{\partial t}\boldsymbol{\omega} + \frac{\partial}{\partial x}\boldsymbol{\kappa} = -\varepsilon \boldsymbol{\omega} \, . \tag{7.9}$$

As expected, symplecticity is not conserved. On the other hand, the perturbed conservation law takes a neat form and suggests that – with increasing time – the average value of symplecticity (i.e. the average of $\boldsymbol{\omega}$ over the spatial domain) is drained out of the field. This suggests thinking about symplecticity as a field variable and studying the implications of its spatial distribution and time dependence, much like the vorticity in a fluid flow.

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