Multi-symplectic spectral discretizations for the Zakharov-Kuznetsov and shallow water equations

Thomas J. Bridges and Sebastian Reich

E-mail: T.Bridges@surrey.ac.uk and S.Reich@surrey.ac.uk

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

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Abstract

The time evolution of multi-symplectic PDEs with periodic boundary conditions in one and two space dimensions is considered. We introduce the idea of a *multi-symplectic Fourier transform* for systems on periodic domains leading to a semi-discretization on Fourier space, and to the concept of multi-symplecticity on Fourier space. We show that this semi-discretization leads automatically to a system of Hamiltonian ODEs in time when truncated, which can be integrated by standard symplectic integrators. We show that the 1D shallow-water equations and the 2D Zakharov-Kuznetsov equation are multi-symplectic and derive spectral discretizations for these systems and present numerical experiments.

1 Introduction

Let us consider a multi-symplectic PDE

$$\mathbf{K}\partial_t \boldsymbol{z} + \mathbf{L}\partial_m \boldsymbol{z} = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}) \tag{1}$$

with independent variables $(t,m) \in \mathbb{R}^2$ and dependent state variable $\boldsymbol{z} \in \mathbb{R}^d$, $d \geq 2$. Here $\mathbf{K}, \mathbf{L} \in \mathbb{R}^{d\times d}$ are two skew-symmetric matrices and $S : \mathbb{R}^d \to \mathbb{R}$ is a scalar-valued smooth function. The system is multi-symplectic in the sense that $\mathbf{K}$ is a skew-symmetric matrix representative of the t direction and $\mathbf{L}$ is a skew-symmetric matrix representative of the m direction, and S represents a Hamiltonian function (cf. [4]).

Associated with the system (1) is a variational equation

$$\mathbf{K}\partial_t Z + \mathbf{L}\partial_m Z = S_{\boldsymbol{zz}}(\boldsymbol{z})Z\,.$$

Take any two solutions U, V of the variational equation, then

$$\partial_t(U^T\mathbf{K}V) + \partial_m U^T\mathbf{L}V) = 0, \tag{2}$$

and, upon introducing the two pre-symplectic forms [3]

$$\omega(U,V) = U^T\mathbf{K}V \qquad \text{and} \qquad \kappa(U,V) = U^T\mathbf{L}V,$$

the equation (2) is equivalent to the conservation law of multi-symplecticity (CLS) [4]

$$\partial_t\omega + \partial_m\kappa = 0. \tag{3}$$

A more abstract approach using wedge product notation [3] yields

$$\omega = \frac{1}{2}\boldsymbol{dz} \wedge \mathbf{K}\boldsymbol{dz} \qquad \text{and} \qquad \kappa = \frac{1}{2}\boldsymbol{dz} \wedge \mathbf{L}\boldsymbol{dz}.$$

There is also an energy conservation law (ECL)

$$\partial_t e + \partial_m f = 0, \tag{4}$$

with energy density

$$e = S(\boldsymbol{z}) - \frac{1}{2}\boldsymbol{z}^T\mathbf{L}(\partial_m \boldsymbol{z})$$

and energy flux

$$f = -\frac{1}{2}(\partial_t \boldsymbol{z})^T\mathbf{L}\boldsymbol{z}.$$

This conservation law is obtained by multiplying (1) with $(\partial_t \boldsymbol{z})^T$ from the right. Similarly, one obtains a momentum conservation law by multiplying (1) with $(\partial_m \boldsymbol{z})^T$ from the right [4].

There is a wide range of partial differential equations that can be formulated as a multi-symplectic PDE (1), including the nonlinear wave equations, KdV-type equations, NLS-type equations, and water waves, for example [4, 5]. Recently, it has been found that the Euler equations in fluid dynamics can be formulated within the framework of multi-symplectic PDEs [6]. In this paper we will show that the 1D shallow water equations [16] – in standard form and regularized – and the Zakharov-Kuznetsov [20] can be formulated as multi-symplectic systems. The Zakharov-Kuznetsov equation is a universal model equation for the effect of weak transverse variation on systems governed by the KdV equation.

Multi-symplecticity is a geometric property of the PDE, and therefore it is natural to require a discretization or semi-discretization to reflect this property. For finite-difference discretizations, some results on this are given in [5], and for Lagrangian first-order field theories in [11]. One of the main results of [5] was that by designing the numerical scheme to conserve symplecticity, the scheme exhibited excellent *local* energy and momentum conservation [12]. While *global* conservation of energy is widely used as a measure of accuracy, *local* energy conservation has rarely been investigated (see however Chapter 6 of [18]). In this paper, we consider the geometric properties of spatial discretizations based on spectral methods. This is the first attempt as far as we are aware to study the multi-symplectic properties of spectral discretizations.

An outline of the paper is as follows. In §§2-3 we present multi-symplectic formulations of the shallow water equations and the Zakharov-Kuznetsov models respectively. In §4 the Fourier transform in the multi-symplectic setting is introduced, and in §5 we show that the associated truncation in Fourier space leads to a system of standard Hamiltonian ODEs which can be discretized in time by a symplectic integration method – see §6. The numerical implementation for the regularized 1D shallow water equations is discussed in §7 while, in §8, the extension of the results to multi-symplectic PDEs (11) with two spatial dimensions (x, y) is outlined and applied to the Zakharov-Kuznetsov equation.

2 Multi-symplectifying 1D shallow-water equations

The one-dimensional shallow water equations are a classic of hydrodynamics, and can be written in the standard form

$$\frac{d}{dt}u = -g\partial_x h, \tag{5}$$

$$\frac{d}{dt}h = -h\partial_x u, \tag{6}$$

where $g > 0$ is a constant representative of gravitational acceleration, $h > 0$ is the fluid layer depth, u is the horizontal fluid velocity and

$$\frac{d}{dt}f = \partial_t f + u\partial_x f$$

denotes the material time derivative of a function f.

These equations are in *Eulerian form.* Their analogous *Lagrangian* form is obtained by letting

$$\frac{d}{dt}x = u, \tag{7}$$

and treating $\frac{d}{dt}$ as a partial derivative (see below). There are a wide range of numerical methods for the Eulerian form particularly with Boussinesq regularization [1]. The Lagrangian form can be discretized using a finite difference approximation for the partial derivative in x, and by introducing a finite dimensional approximation for h. This approach leads to a conservative moving mesh method in the particle locations x. See, for example, [14, 13] and references therein for details.

In this paper, we are interested in a spectral semi-discretization based on a multi-symplectic reformulation of (5)-(7). To multi-symplectify this system, we first introduce the Lagrangian mass coordinate $m \in \mathbb{R}$ which, by definition, satisfies the relation [15, 16]

$$h\gamma = 1, \qquad \gamma = \partial_m x \tag{8}$$

at $t = 0$ and, hence, for all $t \in \mathbb{R}$. Note that (8) replaces the continuity equation (6). Upon transforming the partial derivative ∂_x to the partial derivative ∂_m (which is now the independent spatial variable) and the total time derivative d/dt by the partial derivative ∂_t, we obtain the Lagrangian equations of motion

$$\begin{aligned} \partial_t u &= \partial_m G'(\gamma), \\ \partial_t x &= u, \end{aligned}$$

where $G(\gamma) = g/(2\gamma)$.

It is well-known that the shallow-water equations lead to a steepening of waves and the formation of hydraulic jumps. On the other hand, the addition of dispersion leads to the class of Boussinesq models for shallow water flow. For that reason, we consider the following regularized shallow water equation

$$\partial_t v = \partial_m G'(\gamma), \tag{9}$$

$$(1 - \alpha^2 \partial_m^2)\, \partial_t x = v, \tag{10}$$

where $\alpha \geq 0$ is a small parameter. In Eulerian coordinates, it can be shown that this model is in the equivalence class of Boussinesq models for shallow water flow [6, 9, 19]. It is also related to a shallow-water version of the $\alpha-$Euler model [8].

This regularized system is a Hamiltonian system on a multi-symplectic structure. Expand (9)-(10) as a first order system of PDEs,

$$\begin{aligned} -\partial_t v - \partial_m w &= 0, \\ \partial_t x &= u, \\ \alpha \partial_m s &= v - u, \\ \partial_m x &= \gamma, \\ 0 &= w + G'(\gamma), \\ -\alpha \partial_m u &= s\,. \end{aligned}$$

Then, with state variable $\boldsymbol{z} = (x, v, u, w, \gamma, s)^T \in \mathbb{R}^6$, Hamiltonian

$$S(\boldsymbol{z}) = vu - \frac{1}{2}u^2 + \gamma w + G(\gamma) + \frac{1}{2}s^2,$$

and the pair of skew-symmetric matrices $\mathbf{K}$ and $\mathbf{L}$,

$$\mathbf{K} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{L} = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \alpha \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\alpha & 0 & 0 & 0 \end{pmatrix},$$

the system can be written in the standard form (1).

The conservation law of symplecticity is given by (3) with

$$\omega := dv \wedge dx \qquad \text{and} \qquad \kappa := dw \wedge dx + \alpha du \wedge ds.$$

Similarly, the energy conservation law is given by (4) with energy density

$$e = \frac{1}{2}\left(u^2 + s^2\right) + G(\tau)$$

and energy flux

$$f = uw - \alpha u \partial_t s.$$

See [6] for more details on the multi-symplectic structure of shallow water and other ideal-fluid dynamics models.

3 Multi-symplectifying the Zakharov-Kuznetsov equation

The system (1) can easily be generalized to two spatial dimensions. This yields, for example, a multi-symplectic PDE

$$\mathbf{K}\partial_t \boldsymbol{z} + \mathbf{L}\partial_x \boldsymbol{z} + \mathbf{M}\partial_y \boldsymbol{z} = \boldsymbol{\nabla}_{\boldsymbol{z}} S(\boldsymbol{z}) \tag{11}$$

in the spatial variables $(x, y) \in [-x_o, x_o] \times [-y_o, y_o]$, $x_o, y_o > 0$, and with periodic boundary conditions in x and y. Here $\mathbf{K}, \mathbf{L}, \mathbf{M} \in \mathbb{R}^{d\times d}$ are skew-symmetric matrices, $\boldsymbol{z} \in \mathbb{R}^d$, and $S : \mathbb{R}^d \to \mathbb{R}$ a smooth function. This system has associated conservation laws of symplecticity, energy, and momentum as well which are straightforward generalizations of those given above (cf. [4]).

The Zakharov-Kuznetsov equation [20] is a universal model equation which represents a generalization of the KdV equation to include weak transverse variation,

$$\partial_t u + \partial_x f(u) + \partial_x^3 u + \partial_x \partial_y^2 u = 0, \tag{12}$$

where $f(u)$ can be any scalar smooth function of u, and for definiteness we will take $f(u)$ to be of the form given in the original paper: $f(u) = u^2/2$. This system can be reformulated as a multi-symplectic PDE as follows; (12) is equivalent to the following system of first-order PDEs,

$$\begin{aligned}
\partial_x \phi &= u, && (13)\\
\frac{1}{2}\partial_t \phi + \partial_x v + \partial_y w &= p - f(u), && (14)\\
\partial_x w - \partial_y v &= 0, && (15)\\
-\frac{1}{2}\partial_t u - \partial_x p &= 0, && (16)\\
-\partial_x u + \partial_y q &= -v, && (17)\\
-\partial_x q - \partial_y u &= -w. && (18)
\end{aligned}$$

The state vector is $\boldsymbol{z} = (p, u, q, \phi, v, w) \in \mathbb{R}^6$ and the Hamiltonian function S is given by

$$S = up - \frac{1}{2}\left(v^2 + w^2\right) - F(u),$$

where $f(u) = F'(u)$, $F(u) = u^3/6$. We can assume without loss of generality that $q = 0$ and $2p = f(u) + \partial_x v + \partial_y w$ at $t = 0$ which then holds for all $t \geq 0$.

The conservation law of symplecticity is

$$\partial_t \omega + \partial_x \kappa_1 + \partial_y \kappa_2 = 0,$$

where

$$\omega = \frac{1}{2} du \wedge d\phi, \quad \kappa_1 = dp \wedge d\phi + du \wedge dv + dq \wedge dw \quad \text{and} \quad \kappa_2 = du \wedge dw + dv \wedge dq\,.$$

The energy conservation law is

$$\partial_t e + \partial_x f_1 + \partial_y f_2 = 0, \tag{19}$$

with energy density

$$e = \frac{1}{2}\left(v^2 + w^2\right) - F(u)$$

and the two energy fluxes

$$f_1 = -v\partial_t u - 2p^2 \quad \text{and} \quad f_2 = -w\partial_t u.$$

With periodic boundary conditions over the domain $(x, y) \in [-x_o, x_o] \times [-y_o, y_o]$, the conservation law of energy implies global conservation of the total energy; i.e.,

$$\partial_t E(t) = \partial_t \int_{y=-y_o}^{y_o} \int_{x=-x_o}^{x_o} e \, dxdy = 0\,.$$

Moreover, there is a conservation law for momentum of the form

$$\partial_t m + \partial_x g_1 + \partial_y g_2 = 0,$$

with momentum density

$$m = \frac{1}{2}u^2$$

and the two momentum fluxes

$$g_1 = -F(u) + 2up + \frac{1}{2}\left(w^2 - v^2\right) \quad \text{and} \quad g_2 = -wv.$$

On the periodic box in (x, y), this implies conservation of total momentum; i.e.,

$$\partial_t M(t) = \partial_t \int_{y=-y_o}^{y_o} \int_{x=-x_o}^{x_o} m \, dxdy = 0.$$

See [10] for a complete list of known first integrals for the Zakharov-Kuznetsov equation.

4 The Fourier Transform of a Multi-Symplectic PDE

Let us consider the space of periodic and square integrable functions over the interval $I = [-m_o, m_o]$, $m_o > 0$. We denote this space by $L_2(I)$. The discrete Fourier transform of any function $u \in L_2(I)$ can be written as

$$U = \mathcal{F}u.$$

Here $\mathcal{F} : L_2 \to l_2$ denotes the Fourier operator which gives the complex-valued Fourier coefficients $U_k \in \mathbb{C}$, $k = -\infty, \ldots, -1, 0, 1, \ldots, \infty$, which we collect in the infinite-dimensional vector $U = (\ldots, U_{-1}, U_0, U_1, \ldots) \in l_2$. Note that $U_{-k} = U_k^*$. We also introduce the L_2 inner product, which we denote by (u, v), and the l_2 inner product, which we denote by $\langle U, V\rangle$. The adjoint Fourier operator $\mathcal{F}^* : l^2 \to L^2$ is defined by

$$\langle Z, \mathcal{F}u\rangle = (\mathcal{F}^* Z, u)\,.$$

Since $\mathcal{F}$ is a unitary operator, we have $\mathcal{F}^{-1} = \mathcal{F}^*$.

These definitions can be easily generalized to vector-valued functions $\boldsymbol{z} \in L_2^d(I)$. We use the Kronecker product notation and write the Fourier operator $\widehat{\mathcal{F}} : L_2^d(I) \to l_2^d$ as

$$\widehat{\mathcal{F}} = \mathcal{F} \otimes \mathbf{I}_d,$$

where $\mathbf{I}_d \in \mathbb{R}^{d\times d}$ denotes the $d \times d$ identity matrix. Thus

$$\boldsymbol{Z} = (\mathcal{F} \otimes \mathbf{I}_d)\, \boldsymbol{z}.$$

Let us generalize this notation one step further. We consider now functions $\boldsymbol{z}(t,x)$ that are elements of $L_2^d(I)$ for all $t \in \mathbb{R}$. Then we can write, with a slight abuse of notation,

$$\boldsymbol{z}(t,m) = \widehat{\mathcal{F}^*}(m)\boldsymbol{Z}(t) = (\mathcal{F}^*(m) \otimes \mathbf{I}_d)\,\boldsymbol{Z}(t). \tag{20}$$

Furthermore, partial differentiation with respect to $m \in I$ simply reduces to

$$\partial_m \boldsymbol{z}(t,m) = (\mathcal{F}^*(m)\Theta \otimes \mathbf{I}_d)\boldsymbol{Z}(t),$$

where $\Theta : l_2 \to l_2$ is the diagonal spectral operator with entries

$$\theta_k = \mathtt{i}\frac{\pi k}{m_o}, \quad \mathtt{i} = \sqrt{-1}.$$

We now apply the identity (20) to the multi-symplectic PDE (1). We obtain

$$\mathbf{K}\partial_t(\mathcal{F}^*(m) \otimes \mathbf{I}_d)\boldsymbol{Z}(t) + \mathbf{L}(\mathcal{F}^*(m)\Theta \otimes \mathbf{I}_d)\boldsymbol{Z}(t) = \boldsymbol{\nabla}_{\boldsymbol{z}} S\left(\widehat{\mathcal{F}^*}(m)\boldsymbol{Z}(t)\right).$$

Upon applying the Fourier operator $\widehat{\mathcal{F}} = \mathcal{F} \otimes \mathbf{I}_d$ to this equation, we derive the infinite dimensional system of ordinary differential equations

$$\mathbf{K}\partial_t\boldsymbol{Z} + \mathbf{L}(\Theta \otimes \mathbf{I}_d)\boldsymbol{Z} = \boldsymbol{\nabla}_{\boldsymbol{Z}}\tilde{S}\left(\boldsymbol{Z}\right), \qquad \boldsymbol{Z} \in l_2^n. \tag{21}$$

Here the matrices $\mathbf{K}$, $\mathbf{L} \in \mathbb{R}^{d\times d}$ act component-wise on each Fourier mode $\boldsymbol{Z}_k \in \mathbb{C}^d$ and

$$\tilde{S}(\boldsymbol{Z}) := \int_{-m_o}^{+m_o} S\left(\widehat{\mathcal{F}^*}(m)\boldsymbol{Z}\right)\, dm.$$

Thus we have obtained, what could be called, a multi-symplectic PDE in Fourier space.

We can now look at the associated conservation laws. Upon introducing the Fourier transforms $\Omega := \mathcal{F}\omega \in l_2$ and $\mathcal{K} := \mathcal{F}\kappa \in l_2$, we obtain from (3) the following conservation laws of symplecticity in Fourier space:

$$\partial_t\Omega_k + \theta_k\mathcal{K}_k = 0. \tag{22}$$

This equation is most easily understood in terms of the variational equation associated with (21). Take any two solutions $\boldsymbol{U}, \boldsymbol{V}$ of that linear equation in Fourier space. Then (22) is equivalent to

$$\partial_t\langle\boldsymbol{U}, \mathbf{K}\boldsymbol{V}\rangle + \langle\boldsymbol{U}, \mathbf{L}(\Theta \otimes \mathbf{I}_d)\boldsymbol{V}\rangle + \langle(\Theta \otimes \mathbf{I}_d)\boldsymbol{U}, \mathbf{L}\boldsymbol{V}\rangle = 0. \tag{23}$$

In the same manner; upon introducing the transforms $E := \mathcal{F}e \in l_2$ and $F := \mathcal{F}f \in l_2$, we derive the spectral energy conservation law

$$\partial_t E_k + \theta_k F_k = 0.$$

The formulation of the 1D regularized shallow-water equations in Fourier space is given in §7.

5 A Multi-symplectic Spectral Discretization

To obtain a finite-dimensional spatial discretization, we truncate the higher-order Fourier modes following the usual spectral formulation [7]. However, since the Fourier transform preserves the multi-symplectic structure – indeed, induces a multi-symplectic structure on Fourier space – we obtain a multi-symplectic spatial discretization.

Introduce the discrete Fourier transform $\boldsymbol{\mathcal{F}} : \mathbb{R}^{2N} \to \mathbb{C}^{2N}$ defined by

$$U_k = \frac{1}{\sqrt{2N}}\sum_{l=1}^{2N} u_l e^{-\theta_k(l-1)\Delta m},$$

where

$$\theta_k = \mathrm{i}\frac{\pi(k-1)}{m_o}, \qquad \Delta m = \frac{m_o}{N},$$

and $u_l \approx u(m_l)$, $m_l = -m_o + (l-1)\Delta m$ (cf. [7]). Upon replacing $\widehat{\mathcal{F}^*}$ by $\widehat{\boldsymbol{\mathcal{F}}^*} = \boldsymbol{\mathcal{F}}^* \otimes \mathbf{I}_d$ in (21), we obtain the finite-dimensional system

$$\mathbf{K}\partial_t \boldsymbol{Z} + \mathbf{L}(\bar{\boldsymbol{\Theta}} \otimes \mathbf{I}_d)\boldsymbol{Z} = \boldsymbol{\nabla}_{\boldsymbol{Z}} \bar{S}\,(\boldsymbol{Z}) \tag{24}$$

in the variable $\boldsymbol{Z} = (\boldsymbol{Z}_1, \ldots, \boldsymbol{Z}_{2N}) \in \mathbb{C}^{d\times(2N)}$, where

$$\bar{S}(\boldsymbol{Z}) := \sum_{l=1}^{2N} S\left(\frac{1}{\sqrt{2N}}\sum_{k=1}^{2N} \boldsymbol{Z}_k e^{+\theta_k (l-1)\Delta m}\right)$$

and $\bar{\boldsymbol{\Theta}} \in \mathbb{C}^{2N\times 2N}$ is the diagonal spectral discretization matrix in Fourier space [7]. Let us denote the diagonal entries of $\bar{\boldsymbol{\Theta}}$ by $\bar{\theta}_k$. We have the relation

$$\bar{\theta}_k = \theta_k \quad \text{for} \quad k = 1, \ldots, N,$$

$\bar{\theta}_{N+1} = 0$, and

$$\bar{\theta}_k = -\theta_{2N-k+2} \quad \text{for} \quad k = N+2, \ldots, 2N$$

which follows from the periodicity of the discrete Fourier transform [7].

The Fourier spectral discretization is multi-symplectic in the sense that there is a family of discrete conservation laws of symplecticity which resemble the conservation law (23) in Fourier space. In particular, any pair of solutions $\boldsymbol{U}, \boldsymbol{V}$ to the variational equation associated to (24) satisfy

$$\partial_t \langle \boldsymbol{U}, \mathbf{K}\boldsymbol{V}\rangle + \langle \boldsymbol{U}, \mathbf{L}(\bar{\boldsymbol{\Theta}} \otimes \mathbf{I}_d)\boldsymbol{V}\rangle + \langle (\bar{\boldsymbol{\Theta}} \otimes \mathbf{I}_d)\boldsymbol{U}, \mathbf{L}\boldsymbol{U}\rangle = 0. \tag{25}$$

This discrete conservation law approximates the continuous conservation law (3). Let ω_l and κ_{lk} be pre-symplectic forms, defined by

$$\omega_l := \frac{1}{2}\boldsymbol{dz}_l \wedge \mathbf{K}\boldsymbol{dz}_l \quad \text{and} \quad \kappa_{lk} := \frac{1}{2}\left(\boldsymbol{dz}_l \wedge \mathbf{L}\boldsymbol{dz}_k + \boldsymbol{dz}_k \wedge \mathbf{L}\boldsymbol{dz}_l\right).$$

Then, following (25), the discrete conservation law of symplecticity is given by

$$\partial_t \omega_l + \sum_{k=1}^{2N} d_{lk}\kappa_{lk} = 0\,, \quad \text{where} \quad \boldsymbol{D} = \{d_{lk}\} := \boldsymbol{\mathcal{F}}\bar{\boldsymbol{\Theta}}\boldsymbol{\mathcal{F}}^* \tag{26}$$

is the spectral differentiation matrix [7]. Note that $\boldsymbol{D}$ is a discretization of ∂_x which retains the skew-symmetry property: $\boldsymbol{D}$ is a skew-symmetric matrix.

To verify that the discrete conservation law (26), linearize equation (24) and apply the inverse Fourier transform to obtain

$$\mathbf{K}\partial_t \boldsymbol{dz}_l + \sum_{k=1}^{2N} \mathbf{L} d_{lk}\boldsymbol{dz}_k = S_{\boldsymbol{zz}}(\boldsymbol{z}_l)\,\boldsymbol{dz}_l.$$

Upon taking the wedge product with $\boldsymbol{dz}_l$ and noting that

$$\boldsymbol{dz}_l \wedge S_{\boldsymbol{zz}}(\boldsymbol{z}_l)\,\boldsymbol{dz}_l = 0,$$

the result (26) follows.

One advantage of the multi-symplectic spectral discretization is that is automatically induces a symplectic flow in time. Since $d_{lk} = -d_{kl}$ and $\kappa_{lk} = \kappa_{kl}$, the equation (26) can be summed over the spatial index to obtain

$$\partial_t \sum_{l=1}^{2N} \omega_l = 0,$$

which implies conservation of *total* symplecticity over time.

6 Symplectic Time Integration

The initial value problem (24) can be integrated using a discrete time integration method. (A temporal spectral method can also be used when looking for special solutions such as periodic solutions.) To be consistent a symplectic time integration method should be used, such as the implicit midpoint method, in order to obtain a multi-symplectic integrator [5, 12]. In certain cases a fully explicit symplectic discretization can also be found. In the first example we will show that it is also possible to reformulate the equations in such a way that the explicit symplectic Störmer-Verlet method can be used.

7 Numerical Experiments in 1D: discretized RSW equation

The 1D regularized shallow-water system can be discretized by our spectral method to yield

$$\begin{aligned}
-\partial_t V_k - \bar{\theta}_k W_k &= 0, \\
\partial_t X_k &= U_k, \\
\alpha \bar{\theta}_k S_k &= V_k - U_k, \\
\bar{\theta}_k X_k &= \Gamma_k, \\
0 &= W_k + \nabla_{\Gamma_k} \bar{G}(\mathbf{\Gamma}), \\
-\alpha \bar{\theta}_k U_k &= S_k.
\end{aligned}$$

We compactify this system to a form of a canonical system of Hamiltonian differential equations

$$\begin{aligned}
\frac{d}{dt} V_k &= -\nabla_{X_k} \bar{G}(\bar{\mathbf{\Theta}} \boldsymbol{X}), \\
\frac{d}{dt} X_k &= (1 - \alpha^2 \bar{\theta}_k^2)^{-1} V_k
\end{aligned}$$

with canonical variables $(\boldsymbol{X}, \boldsymbol{U}) \in \mathbb{C}^{2N+1} \times \mathbb{C}^{2N+1}$.

This system is now discretized in time by the explicit and symplectic Störmer-Verlet method [17]. To simplify the notation, we write this method in the non-staggered form

$$\begin{aligned}
V_k^{n+1} &= V_k^n - \Delta t \nabla_{X_k} \bar{G}(\bar{\mathbf{\Theta}} \boldsymbol{X}^n), \\
X_k^{n+1} &= X_k^n + \frac{\Delta t}{1 - \alpha^2 \bar{\theta}_k^2} V_k^{n+1}.
\end{aligned}$$

In order to compute the local energy conservation law (ECL), we also introduce the discrete variables

$$\{\boldsymbol{z}_l^n\} := \widehat{\boldsymbol{\mathcal{F}}} \boldsymbol{Z}^n, \qquad \boldsymbol{z}_l^n \approx \boldsymbol{z}(t_n, x_l),$$

in m-space. Then we define the discrete field of energy densities $e_l^n = e(\boldsymbol{z}_l^n)$ and energy fluxes $f_l^n = f(\boldsymbol{z}_l^n)$. This yields the discrete energy conservation laws

$$\frac{\boldsymbol{E}^{n+1} - \boldsymbol{E}^n}{\Delta t} + \bar{\mathbf{\Theta}} \frac{\boldsymbol{F}^{n+1} + \boldsymbol{F}^n}{2} = \boldsymbol{R}$$

in Fourier space, where $\boldsymbol{E}^n = \boldsymbol{\mathcal{F}}^* \boldsymbol{e}^n$ and $\boldsymbol{e}^n = \{e_l^n\}$ etc. The vector $\boldsymbol{R} \in \mathbb{C}^{2N+1}$ denotes the residual due to *local* non-conservation of energy under numerical discretization. This local error will also be compared with the global energy error.

To test the numerical scheme, we consider the shallow-water equations and the regularized shallow-water equations with periodic boundary conditions and period 1: $\boldsymbol{z}(t, 0) = \boldsymbol{z}(t, 1)$. The initial depth at $t = 0$ is taken to be $h = 1$. The Fourier discretization uses $N = 32$, and the initial velocity field is

$$v(0, m) = 0.1 \sin(2\pi m).$$

The step-size is $\Delta t = 0.0005$. The equations of motion are solved for $\alpha = 0$ (standard shallow-water system: SWS) and $\alpha = 0.01$, $\alpha = 0.05$ respectively (regularized shallow-water system: GSW1 and GSW2). The results can be found in Fig. 1. The top row of graphs in Fig. 1 show the fluid depth h as a function of x at fixed time $t = 2.3$ for the three cases. The regularizing effect of α is evident. The lower row of graphs show the residual of the energy as a function of x at the same time, confirming the excellent energy local energy conservation properties of symplectic and multi-symplectic integrators (cf. [5, 12]).

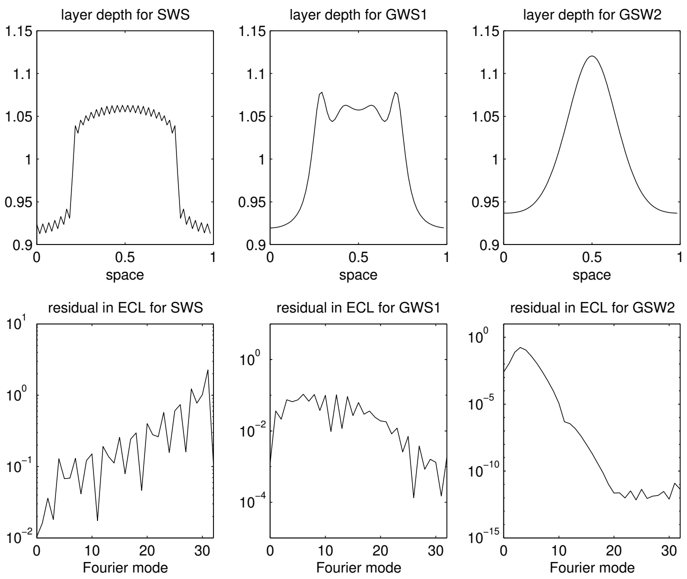

Figure 1: The layer depths and the Fourier transformed residual of the energy conservation law (ECL) at time $t = 2.3$ for $\alpha = 0$ (SSW), $\alpha = 0.01$ (GSW1), and $\alpha = 0.05$ (GSW2).

To investigate the role of α on the Fourier spectrum, we plot the Fourier spectrum for each of the three fluid depths displayed in Fig. 1. The result can be found in Fig. 2. The longer wavelengths show excellent agreement, and at the shorter wavelengths the effect of α regularization is apparent in smoothing out the short wavelengths. We extended the interval of integration to $t \in [0, 100]$ and, for $\alpha = 0.05$, observed no significant changes to the results presented in Figs. 1–2.

8 Numerical experiments in 2D: discretized ZK equation

In this section, the case of spectral discretization of multi-symplectic PDEs in two space dimensions is considered with periodic boundary conditions over the domain $(x, y) = [-m_o, m_o] \times [-m_o, m_o]$, with $m_o > 0$ some constant. The transformation of the multi-symplectic PDE (11) into Fourier space follows the same line as in in §§4-5 for the PDE (1). The truncated system is constructed as follows.

Assume a spatial mesh-size of $\Delta x = \Delta y = m_o/N$ in both directions and introduce the discrete one-dimensional Fourier transform $\boldsymbol{\mathcal{F}} : \mathbb{R}^{2N} \to \mathbb{C}^{2N}$. The discretized state variable over the rectangular mesh is denoted by $\boldsymbol{z}_{kl}(t) \approx \boldsymbol{z}(t, k\Delta x, l\Delta y)$ and its Fourier coefficients by $\boldsymbol{Z}_{kl}$. We have the relation

$$\{\boldsymbol{Z}_{kl}\} = (\boldsymbol{\mathcal{F}} \otimes \mathbf{I}_d)\{\boldsymbol{z}_{kl}\}(\boldsymbol{\mathcal{F}}^T \otimes \mathbf{I}_d).$$

Here $\{\boldsymbol{z}_{kl}\}$ denotes the matrix with vector-valued entries $\boldsymbol{z}_{kl} \in \mathbb{R}^d$ and similarly for $\{\boldsymbol{Z}_{kl}\}$. Thus, using a product construct following the formulation in §5, the spatially discretized system is characterized by

$$\mathbf{K}\partial_t \boldsymbol{Z}_{kl} + \bar{\theta}_k \mathbf{L}\boldsymbol{Z}_{kl} + \bar{\theta}_l \mathbf{M}\boldsymbol{Z}_{kl} = \boldsymbol{\nabla}_{\boldsymbol{Z}_{kl}} \bar{S}(\boldsymbol{Z})$$

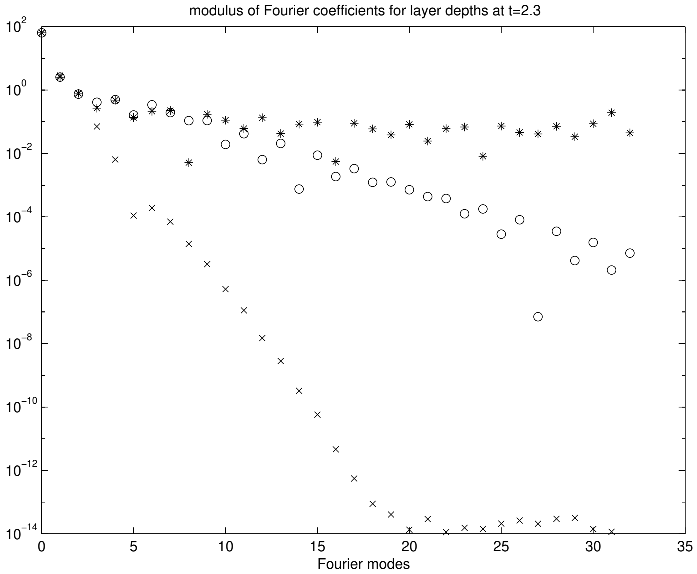

Figure 2: The modulus of the Fourier modes of the layer depths at $t = 2.3$ for $\alpha = 0$ (SWS *), $\alpha = 0.01$ (GSW1 o), and $\alpha = 0.05$ (GSW2 x).

where $\boldsymbol{Z} = \{\boldsymbol{Z}_{kl}\}$ and

$$\bar{S}(\boldsymbol{Z}) = \sum_{i,j=1}^{2N} S\left(\frac{1}{2N}\sum_{k,l=1}^{2N} \boldsymbol{Z}_{kl} e^{+\theta_k (i-1)\Delta x} e^{+\theta_l (j-1)\Delta y}\right).$$

The frequencies θ_k and $\bar{\theta}_k$ are as defined in §5.

In the remainder of this section, we use this formulation to study a Fourier spectral discretization of Zakharov-Kuznetsov equation in its multi-symplectic formulation (13)-(18). The Fourier transform and truncation leads to

$$\begin{aligned}
\bar{\theta}_k \Phi_{kl} &= U_{kl}, \\
\frac{1}{2}\partial_t \Phi_{kl} + \bar{\theta}_k V_{kl} + \bar{\theta}_l W_{kl} &= P_{kl} - \nabla_{U_{kl}} \bar{F}(\boldsymbol{U}), \\
\bar{\theta}_k W_{kl} - \bar{\theta}_l V_{kl} &= 0, \\
-\frac{1}{2}\partial_t U_{kl} - \bar{\theta}_k P_{kl} &= 0, \\
-\bar{\theta}_k U_{kl} + \bar{\theta}_l Q_{kl} &= -V_{kl}, \\
-\bar{\theta}_k Q_{kl} - \bar{\theta}_l U_{kl} &= -W_{kl}.
\end{aligned}$$

Without loss of generality, we can assume that $Q_{kl} = 0$ and

$$2P_{kl} = \nabla_{U_{kl}} \bar{F}(\boldsymbol{U}) + \bar{\theta}_k V_{kl} + \bar{\theta}_l W_{kl}$$

at $t = 0$ which then holds for all $t \geq 0$. Thus the discrete Fourier system can be compactified to

$$\partial_t U_{kl} + \bar{\theta}_k \left(\nabla_{U_{kl}} \bar{F}(\boldsymbol{U}) + \bar{\theta}_k^2 U_{kl} + \bar{\theta}_l^2 U_{kl}\right) = 0$$

which in fact recovers a standard spectral discretization applied directly to the ZK equation. Therefore, our discrete system of ODEs recovers that in [10]. This discrete system of ODEs is Hamiltonian and should therefore be integrated in time by the symplectic method [17]. Here we will use the implicit midpoint rule.

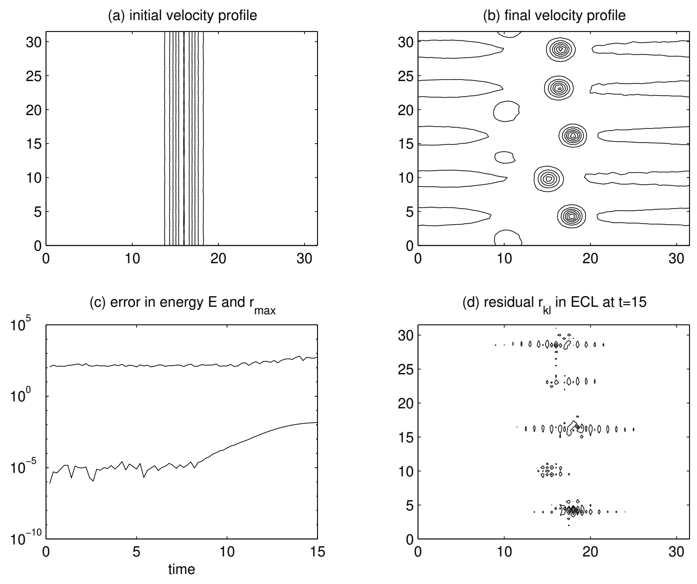

Figure 3: Numerical results for the Zakharov-Kuznetsov equation.

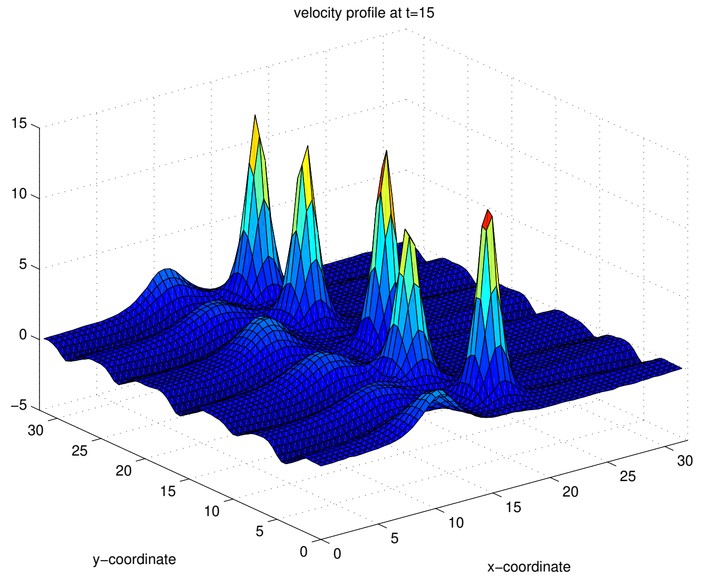

Figure 4: Cylindrical soliton pulses at time $t = 15$ for ZK simulation.

To test the algorithm, we repeated one of the numerical experiments as reported in [10]. We simulated the transverse instability of a 1D solitary wave (cf. [2] and references therein), and its subsequent breakup into cylindrical solitons. We started the simulation with the perturbed soliton

$$u(x, y, 0) = 3c\,\mathrm{sech}^2(0.5\sqrt{c}(x - 16)) + \xi(x, y), \quad c = 2,$$

where $\xi(x, y)$ is a random perturbation. The numerical results are shown in Fig. 3. These results are in qualitative agreement with the computations in [10].

As a numerical check, we monitored the error

$$\Delta E(t_n) = |E(t_n) - E(0)|$$

in the total energy of the system and the numerically induced residual $r_{kl}(t_n)$ in the energy conservation law (19) for each grid point (x_k, y_l).[1] Note the relation

$$\frac{E(t_n) - E(t_{n-1})}{\Delta t} = \sum_{kl} r_{kl}(t_n).$$

We found that the total energy is well behaved as a function of time: see the lower curve in Fig. 3(c). However $r_{max}(t_n) = \max|r_{kl}(t_n)|$ the residual in the energy conservation law is large: see the upper curve in Fig. 3(c)). The local ECL error is greatest near the cylindrical solitions: see Fig. 3(d)). This error is due to the fact that $2N = 64$ which corresponds to a mesh size of $\Delta x = \Delta y = 0.5$. This mesh size is relatively coarse compared to the width of the initial soliton and the cylindrical solitons formed later: see Fig. 4. (Initial tests show that the local ECL error decreases when a finer mesh is used.) The height of the cylindrical pulses is $U_{max} \approx 14.0574$ which indicates that the velocity is about $c = 2.97$. Therefore, although the *global* energy is conserved very well with the coarse discretization, the local ECL error can have large fluctuations – but this is a useful indicator of spatial discretization errors. This is one of the advantages of the multi-symplectic discretization where the ECL is a natural part of the discretization.

References

[1] M. B. Abbott & D. R. Basco, *Computational Fluid Dynamics*, Longman Scientific, 1989.

[2] M. A. Allen & G. Rowlands, *Determination of the growth rate for the linearized Zakharov-Kuznetsov equation*, J. Plasma Phys. **50**, 1993, 413–424.

[3] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer-Verlag, 1978.

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

[5] T. J. Bridges & S. Reich, *Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity*, UniS Preprint; submitted, 1999.

[6] T. J. Bridges & S. Reich, *The multi-symplectic geometry of ideal fluids and conservative integration methods*, in preparation.

[7] B. Fornberg, *A Practical Guide to Pseudospectral Methods*, Cambridge University Press, 1996.

[8] D. D. Holm, J. E. Marsden & T. S. Ratiu, *Euler-Poincaré models for ideal fluids with nonlinear dispersion*, Phys. Rev. Lett. **349** (1998), 4173–4177.

[9] E. Infeld & G. Rowlands, *Nonlinear Waves, Solitons and Chaos*, Cambridge University Press, Cambridge, 1990.

[10] H. Iwasaki, S. Toh & T. Kawahara, *Cylindrical quasi-solitons to the Zakharov-Kuznetsov equations*, Physica D **43** (1990), 293–303.

[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] S. Reich, *Multi-symplectic Runge-Kutta collocation methods for Hamiltonian wave equations*, J. Comput. Phys. **157** (2000), 473–499.

[13] S. Reich, *The repulsive-particle method and the symplectic integration of the shallow-water equations*, UniS Preprint, 1999.

[1] The residuals $r_{kl}(t_n)$ were computed in a similar manner as described in §7. We first computed the Fourier transform $\boldsymbol{R}$ of the residual and then transformed back to coordinate space.

[14] R. D. Richtmeyer & K. W. Morton, *Difference Methods for Initial-Value Problems*, Interscience, New York, 1967.

[15] W. van Saarloos, *A canonical transformation relating the Lagrangian and Eulerian description of ideal hydrodynamics*, Physica **108A** (1981), 557–566.

[16] R. Salmon, *Lectures on Geophysical Fluid Dynamics*, Oxford University Press, Oxford, 1999.

[17] J. M. Sanz-Serna & M. P. Calvo, *Numerical Hamiltonian Systems*, Chapman & Hall, London, 1994.

[18] R. Vichnevetsky & J. B. Bowles, *Fourier Analysis of Numerical Approximations of Hyperbolic Equations*, SIAM: Philadelphia, 1982.

[19] G. B. Whitham, *Linear and Nonlinear Waves*, John Wiley & Sons, 1974.

[20] V. E. Zakharov & E. A. Kuznetsov, *Three-dimensional solitons*, Sov. Phys. JETP **39** (1974), 285–286.