Conservation of wave action by multisymplectic Runge-Kutta box schemes

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Abstract. In this note we show that multisymplectic Runge-Kutta box schemes, of which the Gauss-Legendre methods are the most important, preserve a discrete conservation law of wave action. The result follows by loop integration over an ensemble of flow realizations, and the local energy-momentum conservation law for continuous variables in semi-discretizations.

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1. Introduction

The conservation of wave action was introduced in (Whitham 1965) for slow modulations of traveling wave trains. The concept was further extended in (Whitham 1970) (see also (Whitham 1999)). Whitham's theory has found application in wave-mean field interactions (Andrews & McIntyre 1978), (Grimshaw 1984) and instability theory (see (Bridges 1997*b*, Bridges 1997*a*) and the references therein). The most general form of the conservation law of wave action was introduced by (Hayes 1970), and it is this form that will be treated here, using the multisymplectic formalism of (Bridges 1997*a*). Hayes's approach to wave action conservation was to consider a periodic, one-parameter family of solutions to the Euler-Lagrange equations. The wave action conservation law then follows from Noether's theorem, due to the trivial invariance of the action integral under translations in the ensemble parameter. The identification of the ensemble parameter with a phase shift recovers Whitham's theory, and it is clear that the importance of this conservation law is that it holds even when the action integral is explicitly dependent on time and space, such that the energy-momentum tensor is not exactly conserved. The local conservation law for wave action is a space-time generalization of the concept of an adiabatic invariant in a classical mechanical system with slow dependence of the Hamiltonian on time (Arnold 1989). Wave action with multiple ensemble parameters is considered in (Hayes 1970) and (Ablowitz & Benney 1970).

Consider an abstract Hamiltonian PDE in multisymplectic form (Bridges 1997*b*)

$$K\partial_t \boldsymbol{u} + L\partial_x \boldsymbol{u} = \nabla S(\boldsymbol{u}, t, x), \qquad (1)$$

where $\boldsymbol{u}(t,x) \in \boldsymbol{R}^N$, $K^T = -K$ and $L^T = -L$ are $N \times N$ skew-symmetric matrices, and $S : \boldsymbol{R}^N \times \boldsymbol{R} \times \boldsymbol{R} \to \boldsymbol{R}$ is a functional, which may depend on t and x. Consider a one-parameter ensemble of solutions $\boldsymbol{u}(t,x,\theta)$ depending smoothly on $\theta \in \mathcal{S}^1$. Taking the vector inner product of (1) with $\partial_\theta \boldsymbol{u}$ yields the conservation law

$$\partial_\theta \left(\frac{1}{2}\langle K\partial_t \boldsymbol{u}, \boldsymbol{u}\rangle + \frac{1}{2}\langle L\partial_x \boldsymbol{u}, \boldsymbol{u}\rangle - S(\boldsymbol{u},t,x) \right) + \partial_t (\frac{1}{2}\langle K\boldsymbol{u}, \partial_\theta \boldsymbol{u}\rangle) + \partial_x(\frac{1}{2}\langle L\boldsymbol{u}, \partial_\theta \boldsymbol{u}\rangle) = 0,$$

as can be checked (Bridges 1997*a*). The ensemble average gives Hayes's conservation law of wave action

$$\partial_t \mathcal{A} + \partial_x \mathcal{B} = 0, \quad \mathcal{A} = \oint \frac{1}{2}\langle K\boldsymbol{u}, \partial_\theta \boldsymbol{u}\rangle \, d\theta, \quad \mathcal{B} = \oint \frac{1}{2}\langle L\boldsymbol{u}, \partial_\theta \boldsymbol{u}\rangle \, d\theta.$$

Multisymplectic numerical discretizations in the sense of (Bridges & Reich 2001) satisfy a discrete conservation law of wave action. This result is a corollary to the result that multisymplectic semi-discretizations satisfy a semi-discrete energy-momentum conservation in each continuous (i.e. undiscretized) independent variable, which follows from the Noether theory for multisymplectic PDEs (Bridges 1997*b*). The latter result has been shown for special cases in the literature (Reich 2000*b*), but the general case has not been recorded. At any rate, the conservation of wave action is therefore not too surprising. The purpose of this paper is to explicitly state the wave action conservation law for one class of MS discretizations, namely the Runge-Kutta box schemes, for an arbitrary number of dimensions and ensemble parameters. We give explicit formulas for the set of conservation laws for undiscretized dimensions, and specify the wave action conservation law by loop integration over the ensemble parameters. Although the result follows from Noether's theory, we derive it directly here based on the symplecticity condition for Runge-Kutta methods, because such an approach yields local conservation laws.

2. Multisymplectic structure and conservation laws

Consider a d-dimensional space-time, with coordinates $\boldsymbol{x} \in \boldsymbol{R}^d$, and phase space $\boldsymbol{R}^N$. A multisymplectic PDE on $\boldsymbol{R}^N$ is written (Bridges 1997*b*)

$$\sum_{\alpha=1}^{d} J^{(\alpha)} \partial_{x_\alpha} \boldsymbol{u}(\boldsymbol{x}) = \nabla S(\boldsymbol{u}, \boldsymbol{x}), \tag{2}$$

where $S : \boldsymbol{R}^N \times \boldsymbol{R}^d \to \boldsymbol{R}$ is a smooth functional and the $J^{(\alpha)}$, $\alpha = 1, \ldots, d$ are $N \times N$ constant skew-symmetric matrices

$$J^{(\alpha)} = -{J^{(\alpha)}}^T$$

with associated presymplectic two-forms

$$\Omega^{(\alpha)}(U,V) = \langle J^{(\alpha)}U, V\rangle, \qquad \forall U, V \in \boldsymbol{R}^N,$$

where $\langle \cdot, \cdot \rangle$ is the standard inner product on $\boldsymbol{R}^N$.

2.1. *Energy-momentum conservation laws*

Taking the inner product of (2) with $\partial_{x_\beta} \boldsymbol{u}(\boldsymbol{x})$ gives

$$\sum_{\alpha=1}^{d} \Omega^{(\alpha)}(\partial_{x_\alpha} \boldsymbol{u}(\boldsymbol{x}), \partial_{x_\beta} \boldsymbol{u}(\boldsymbol{x})) = \langle \nabla S(\boldsymbol{u}, \boldsymbol{x}), \partial_{x_\beta} \boldsymbol{u}(\boldsymbol{x})\rangle. \tag{3}$$

Using the skew-symmetry of $\Omega^{(\alpha)}$, $\Omega^{(\alpha)}(\partial_{x_\beta}\boldsymbol{u}(\boldsymbol{x}), \partial_{x_\beta}\boldsymbol{u}(\boldsymbol{x})) = 0$, and furthermore

$$\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{u}(\boldsymbol{x}), \partial_{x_\beta}\boldsymbol{u}(\boldsymbol{x})) = \partial_{x_\alpha}\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{u}(\boldsymbol{x}), \partial_{x_\beta}\boldsymbol{u}(\boldsymbol{x})) + \partial_{x_\beta}\frac{1}{2}\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{u}(\boldsymbol{x}), \boldsymbol{u}(\boldsymbol{x})).$$

If in addition, $S(\boldsymbol{u}, \boldsymbol{x})$ does not depend explicitly on the coordinate x_β, then $\partial_\beta S(\boldsymbol{u}, \boldsymbol{x}) = \langle \nabla S, \partial_\beta \boldsymbol{u} \rangle$, and it follows that (3) is equivalent to the conservation law (Bridges 1997*b*)

$$\partial_{x_\beta} e_\beta(\boldsymbol{x}) + \sum_{\alpha=1,\alpha\neq\beta}^{d} \partial_{x_\alpha} f_\beta^\alpha(\boldsymbol{x}) = 0 \tag{4}$$

where

$$e_\beta(\boldsymbol{x}) = \sum_{\alpha=1,\alpha\neq\beta}^{d} \frac{1}{2}\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{u}(\boldsymbol{x}), \boldsymbol{u}(\boldsymbol{x})) - S(\boldsymbol{u}(\boldsymbol{x}))$$

$$f_\beta^\alpha(\boldsymbol{x}) = \frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{u}(\boldsymbol{x}), \partial_{x_\beta}\boldsymbol{u}(\boldsymbol{x}))$$

In total there is one such conservation law for each coordinate for which there is no explicit dependence of S. These conservation laws are the momentum maps associated with the translation symmetry in the respective direction (Bridges 1997*b*). For $x_\beta = t$ the time, this is the energy conservation law.

2.2. Conservation of wave action

The wave action conservation principle of (Hayes 1970) has been cast in multisymplectic form in (Bridges 1997*a*). The idea is to consider a family of solutions smoothly parameterized by a closed loop in phase space. We write $\boldsymbol{u}(\boldsymbol{x}, \theta)$ for $\theta \in \mathcal{S}^1$, and compute the inner product of (2) with $\partial_\theta \boldsymbol{u}$:

$$\sum_{\alpha=1}^{d} \Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{u}(\boldsymbol{x}, \theta), \partial_\theta \boldsymbol{u}(\boldsymbol{x}, \theta)) = \langle \nabla S(\boldsymbol{u}, \boldsymbol{x}), \partial_\theta \boldsymbol{u}(\boldsymbol{x}, \theta) \rangle.$$

Using the same reasoning as in the previous section, this yields a conservation law

$$\partial_\theta \mathfrak{a}(\boldsymbol{x}, \theta) + \sum_{\alpha=1}^{d} \partial_{x_\alpha} \mathfrak{b}^\alpha(\boldsymbol{x}, \theta) = 0, \tag{5}$$

where

$$\mathfrak{a}(\boldsymbol{x}, \theta) = \sum_{\alpha=1}^{d} \frac{1}{2}\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{u}(\boldsymbol{x}, \theta), \boldsymbol{u}(\boldsymbol{x}, \theta)) - S(\boldsymbol{u}(\boldsymbol{x}, \theta), \boldsymbol{x})$$

$$\mathfrak{b}^\alpha(\boldsymbol{x}, \theta) = \frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{u}(\boldsymbol{x}, \theta), \partial_\theta \boldsymbol{u}(\boldsymbol{x}, \theta)).$$

Usually, the solution is averaged around the loop to yield the *conservation of wave action*

$$\sum_{\alpha=1}^{d} \partial_{x_\alpha} \mathcal{B}^\alpha = 0, \tag{6}$$

where the wave action α-flux density $\mathcal{B}^\alpha$ is given by

$$\mathcal{B}^\alpha = \oint_{\mathcal{S}^1} \mathfrak{b}^\alpha(\boldsymbol{x}, \theta)\, d\theta.$$

In general there is no reason to restrict oneself to a single ensemble parameter. The case of multiple parameters is also considered by (Hayes 1970) and (Ablowitz & Benney 1970). Note that the conservation law (5) can also be obtained as a special case of (4), by identifying one coordinate, say x_d, with θ and defining a trivial presymplectic form: $J^{(d)} = 0$. Since $S(\boldsymbol{u}, \boldsymbol{x})$ constructed in this way will not depend on x_d, a conservation law (4) associated with translation symmetry in x_d will hold. In the same way we can derive wave action conservation for any number of ensemble parameters, directly from the conservation law (4).

In (Bridges 1997*a*) it is shown that a local conservation law of symplecticity can be derived by applying Stokes theorem to (6). The defining property of a multisymplectic discretization is that it satisfies a discrete version of the local conservation law of symplecticity. Given the above relation between the wave action and symplectic conservation laws, one may expect there to be a discrete conservation law of wave action for multisymplectic integrators. In the next section we identify such a conservation law for the class of multisymplectic Runge-Kutta methods.

3. Wave action conservation for multisymplectic Runge-Kutta box schemes

3.1. Multisymplectic Runge-Kutta discretizations

We consider a semi-discretization of (2) on a tensor-product grid. It is sufficient to consider a single grid cell of dimension $\Delta x_1 \times \cdots \times \Delta x_{d^*}$, $d^* \leq d$, where the equations will be left continuous in the coordinates $(x_{d^*+1}, \ldots, x_d)$. We will assume that $S(\boldsymbol{u}, \boldsymbol{x}) = S(\boldsymbol{u}, x_1, \ldots, x_{d^*})$, so that conservations laws (4) hold for each of the continuous coordinate directions.

For each coordinate direction x_α, $\alpha = 1, \ldots, d^*$, we associate an s^α-stage Runge-Kutta method with coefficients (Hairer et al. 1993) denoted

$$c_j^\alpha, b_j^\alpha, a_{jk}^\alpha, \quad j, k = 1, \ldots, s^\alpha \tag{7}$$

Additionally, we define index sets associated with stage abscissae:

$$\begin{aligned} P^\alpha &= \{1, \ldots, s^\alpha\}, \\ \mathbb{P} &= \prod_{\alpha=1}^{d^*} P^\alpha = \{(i_1, \ldots, i_{d^*}) \,|\, i_\alpha \in P^\alpha\}, \\ \mathbb{Q}^\alpha &= \prod_{\beta=1, \beta\neq\alpha}^{d^*} P^\beta = \{(j_1, \ldots, j_{\alpha-1}, \emptyset, j_{\alpha+1}, \cdots, j_{d^*}) \in \mathbb{P} \,|\, j_\beta \in P^\beta\}. \end{aligned}$$

Note that by our definition the set $\mathbb{Q}^\alpha$ is the subset of $\mathbb{P}$ consisting of those ordered d^*-tuples whose αth element is the null set. This is to preserve the ordering of indices. Given an element $J \in \mathbb{Q}^\alpha$ and an element $k \in P^\alpha$, we denote by $(J; k)$ the element in $\mathbb{P}$ given by $(j_1, \ldots, j_{\alpha-1}, k, j_{\alpha+1}, \ldots, j_{d^*})$.

For $I \in \mathbb{P}$, define the collocation point $\boldsymbol{x}_I = (c_{i_1}^1, \ldots, c_{i_{d^*}}^{d^*}, x_{d^*+1}, \ldots, x_d)$.

With these definitions, the Runge-Kutta box scheme semi-discretization is defined by

$$\sum_{\alpha=1}^{d^*} J^{(\alpha)} \boldsymbol{U}_I^{x_\alpha} + \sum_{\alpha=d^*+1}^{d} J^{(\alpha)} \partial_{x_\alpha} \boldsymbol{U}_I = \nabla S(\boldsymbol{U}_I, \boldsymbol{x}_I), \quad \forall I \in \mathbb{P} \tag{8}$$

where $\boldsymbol{U}_I = \boldsymbol{U}_I(x_{d^*+1}, \ldots, x_d)$, and $\boldsymbol{U}_I^{x_\alpha}$ is a stage vector approximating $\partial_{x_\alpha} \boldsymbol{u}$ at the collocation point $\boldsymbol{x}_I$. Additionally we have the relations

$$\boldsymbol{U}_{(J;j)} = \boldsymbol{u}_J^{\alpha,0} + \Delta x_\alpha \sum_{k=1}^{s^\alpha} a_{jk}^\alpha \boldsymbol{U}_{(J;k)}^{x_\alpha}, \qquad \begin{array}{l} \forall j \in P^\alpha, \\ \forall J \in \mathbb{Q}^\alpha, \\ \alpha = 1, \ldots, d^*. \end{array} \tag{9}$$

In (9) each N-dimensional stage vector on the left side appears in d^* relations, corresponding to a quadrature in each coordinate direction. The quantities $\boldsymbol{u}_J^{\alpha,0}$ and $\boldsymbol{u}_J^{\alpha,1}$ approximate $\boldsymbol{u}$ on the abscissa set $\mathbb{Q}^\alpha$ on the lower and upper α-faces of the grid cell respectively. They are related by

$$\boldsymbol{u}_J^{\alpha,1} = \boldsymbol{u}_J^{\alpha,0} + \Delta x_\alpha \sum_{j=1}^{s^\alpha} b_j^\alpha \boldsymbol{U}_{(J;j)}^{x_\alpha}, \qquad \begin{array}{l} \forall J \in \mathbb{Q}^\alpha, \\ \alpha = 1, \ldots, d^*. \end{array} \tag{10}$$

Additional formulas are necessary to relate the above quantities to gridpoint values (Frank et al. 2005). However, the relations (8), (9) and (10) are sufficient to obtain the conclusions of this paper.

A Runge-Kutta box scheme is multisymplectic (i.e. satisfies a discrete local conservation law of symplecticity in the sense of (Bridges & Reich 2001)) if each coefficient set $\{c_j^\alpha, b_j^\alpha, a_{jk}^\alpha\}$ defines a symplectic RK method (Hairer et al. 2002):

$$b_i^\alpha b_j^\alpha - b_j^\alpha a_{ji}^\alpha - b_i^\alpha a_{ij}^\alpha = 0. \tag{11}$$

3.2. Semi-discrete energy-momentum conservation laws

We are interested in the remnants of the conservation laws (4) after (semi-) discretization.

The following lemma expresses an identity that is crucial for the derivation of semi-discrete conservation laws and the conservation of wave action.

Lemma 1 *Consider a presymplectic two-form Ω and a set of vectors $\boldsymbol{u}^0(\theta)$, $\boldsymbol{u}^1(\theta)$, $\boldsymbol{U}_i(\theta)$, $\boldsymbol{U}_i^x(\theta) \in \boldsymbol{R}^N$, $i = 1, \ldots, s$, smoothly dependent on a parameter θ and satisfying the Runge-Kutta formulas*

$$\boldsymbol{U}_i = \boldsymbol{u}^0 + \Delta x \sum_{j=1}^{s} a_{ij} \boldsymbol{U}_j^x, \quad i = 1, \ldots, s \tag{12}$$

$$\boldsymbol{u}^1 = \boldsymbol{u}^0 + \Delta x \sum_{i=1}^{s} b_i \boldsymbol{U}_j^x. \tag{13}$$

For symplectic Runge-Kutta methods (11) the following identity holds:

$$\sum_{i=1}^{s} b_i \Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_i) = \partial_\theta \left[\sum_{i=1}^{s} b_i \frac{1}{2} \Omega(\boldsymbol{U}_i^x, \boldsymbol{U}_i) \right] + \frac{1}{\Delta x}(F^1 - F^0), \tag{14}$$

with $F^j = \frac{1}{2}\Omega(\boldsymbol{u}^j, \partial_\theta \boldsymbol{u}^j)$, $j = 0, 1$.

Proof. Substitute (13) into the definition of F^1 to obtain

$$\Omega(\boldsymbol{u}^1, \partial_\theta \boldsymbol{u}^1) = \Omega(\boldsymbol{u}^0, \partial_\theta \boldsymbol{u}^0) + \Delta x \sum_{i=1}^{s} b_i \Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{u}^0) + \Delta x \sum_{i=1}^{s} b_i \Omega(\boldsymbol{u}^0, \partial_\theta \boldsymbol{U}_i^x)$$
$$+ \Delta x^2 \sum_{i,j=1}^{s} b_i b_j \Omega(\boldsymbol{U}_j^x, \partial_\theta \boldsymbol{U}_i^x). \tag{15}$$

Solving (12) for $\boldsymbol{u}^0$ (for each i), differentiating with respect to θ, and substituting into the first sum above yields

$$\begin{aligned}\sum_{i=1}^{s} b_i\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{u}^0) &= \sum_{i=1}^{s} b_i\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_i) - \sum_{i,j=1}^{s} b_i a_{ij}\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_j^x) \\ &= \sum_{i=1}^{s} b_i\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_i) - \sum_{i,j=1}^{s} b_j a_{ji}\Omega(\boldsymbol{U}_j^x, \partial_\theta \boldsymbol{U}_i^x),\end{aligned}$$

where the skew-symmetry of the two-form has been used. Similarly, the second sum becomes

$$\sum_{i=1}^{s} b_i\Omega(\boldsymbol{u}^0, \partial_\theta \boldsymbol{U}_i^x) = \sum_{i=1}^{s} b_i\Omega(\boldsymbol{U}_i, \partial_\theta \boldsymbol{U}_i^x) - \sum_{i=1}^{s} b_i a_{ij}\Omega(\boldsymbol{U}_j^x, \partial_\theta \boldsymbol{U}_i^x).$$

Substituting the above two formulas into (15) gives

$$\begin{aligned}\Omega(\boldsymbol{u}^1, \partial_\theta \boldsymbol{u}^1) = \Omega(\boldsymbol{u}^0, \partial_\theta \boldsymbol{u}^0) &+ \Delta x \sum_{i=1}^{s} b_i\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_i) + \Delta x \sum_{i=1}^{s} b_i\Omega(\boldsymbol{U}_i, \partial_\theta \boldsymbol{U}_i^x) \\ &+\Delta x^2 \sum_{i,j=1}^{s} (b_i b_j - b_j a_{ji} - b_i a_{ij})\Omega(\boldsymbol{U}_j^x, \partial_\theta \boldsymbol{U}_i^x). \qquad (16)\end{aligned}$$

For symplectic RK methods (11), the last term in (16) cancels. Finally we note that

$$\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_i) + \Omega(\boldsymbol{U}_i, \partial_\theta \boldsymbol{U}_i^x) = 2\Omega(\boldsymbol{U}_i^x, \partial_\theta \boldsymbol{U}_i) - \partial_\theta \Omega(\boldsymbol{U}_i^x, \boldsymbol{U}_i),$$

and (14) easily follows. □

Let us define the quadrature operator acting on functions $\boldsymbol{U}_I$ defined at the the collocation points $\boldsymbol{x}_I$:

$$\begin{aligned}\mathcal{Q}[S(\boldsymbol{U}_I, \boldsymbol{x}_I)] &:= |\Delta \boldsymbol{x}| \sum_{I\in\mathbb{P}} b_I S(\boldsymbol{U}_I, \boldsymbol{x}_I), \\ \mathcal{Q}[\Omega(\boldsymbol{U}_I, \boldsymbol{V}_I)] &:= |\Delta \boldsymbol{x}| \sum_{I\in\mathbb{P}} b_I \Omega(\boldsymbol{U}_I, \boldsymbol{V}_I),\end{aligned}$$

where $|\Delta \boldsymbol{x}| = \Delta x_1 \Delta x_2 \cdots \Delta x_{d^*}$ and for an element $I \in \mathbb{P}$, $I = (i_1, \ldots, i_{d^*})$, we define $b_I = b^1_{i_1} b^2_{i_2} \cdots b^{d^*}_{i_{d^*}}$.

We also define a quadrature operator over an α-face of the grid cell

$$\mathcal{Q}^\alpha[\Omega(\boldsymbol{u}_J^0, \boldsymbol{v}_J^0)] = \frac{|\Delta \boldsymbol{x}|}{\Delta x_\alpha} \sum_{J\in\mathbb{Q}^\alpha} b_J \Omega(\boldsymbol{u}_J^0, \boldsymbol{v}_J^0),$$

where for $J \in \mathbb{Q}^\alpha$ we define $b_J = b^1_{j_1} \cdots b^{\alpha-1}_{j_{\alpha-1}} \cdot b^{\alpha+1}_{j_{\alpha+1}} \cdots b^{d^*}_{j_{d^*}}$.

Using these definitions we have the following

Theorem 1 *Consider the multisymplectic Runge-Kutta box scheme semi-discretization (8), (9), (10), in which the coordinates $x_1, \ldots, x_d^*$ are discretized and the remaining coordinates are left continuous. Then for each $\beta \in \{d^*+1, \ldots, d\}$, the semi-discrete conservation law holds:*

$$\partial_{x_\beta} e_\beta + \sum_{\alpha=d^*+1, \alpha\neq\beta}^{d} \partial_{x_\alpha} f_\beta^\alpha + \sum_{\alpha=1}^{d^*} \frac{1}{\Delta x_\alpha}(F_\beta^{\alpha,1} - F_\beta^{\alpha,0}) = 0, \qquad (17)$$

where $e(x_{d^*+1},\ldots,x_d)$*,* $f^\alpha_\beta(x_{d^*+1},\ldots,x_d)$*, and* $F^{\alpha,j}_\beta(x_{d^*+1},\ldots,x_d)$*,* $j = 0,1$ *are defined by*

$$e_\beta = \sum_{\alpha=1}^{d^*} \mathcal{Q}\left[\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{U}_I^{x_\alpha}, \boldsymbol{U}_I)\right] + \sum_{\alpha=d^*+1,\alpha\neq\beta}^{d} \mathcal{Q}\left[\frac{1}{2}\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{U}_I, \boldsymbol{U}_I)\right] - \mathcal{Q}[S(\boldsymbol{U}_I, \boldsymbol{x}_I)], \tag{18}$$

$$f^\alpha_\beta = \mathcal{Q}\left[\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{U}_I, \partial_{x_\beta}\boldsymbol{U}_I)\right], \tag{19}$$

$$F^{\alpha,j}_\beta = \Delta x_\alpha \mathcal{Q}^\alpha\left[\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{u}^j_J, \partial_{x_\beta}\boldsymbol{u}^j_{\boldsymbol{J}})\right], \quad j = 1, 2. \tag{20}$$

Proof. Take the inner product of (8) with $\partial_{x_\beta}\boldsymbol{U}_I$,

$$\sum_{\alpha=1}^{d^*}\Omega^{(\alpha)}(\boldsymbol{U}_I^{x_\alpha}, \partial_{x_\beta}\boldsymbol{U}_I) + \sum_{\alpha=d^*+1}^{d}\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{U}_I, \partial_{x_\beta}\boldsymbol{U}_I) - \langle\nabla S(\boldsymbol{U}_I, \boldsymbol{x}_I), \partial_{x_\beta}\boldsymbol{U}_I\rangle = 0,$$

and apply the quadrature operator $\mathcal{Q}$ to each term

$$\sum_{\alpha=1}^{d^*}\mathcal{Q}[\Omega^{(\alpha)}(\boldsymbol{U}_I^{x_\alpha}, \partial_{x_\beta}\boldsymbol{U}_I)] + \sum_{\alpha=d^*+1}^{d}\mathcal{Q}[\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{U}_I, \partial_{x_\beta}\boldsymbol{U}_I)] - \mathcal{Q}[\partial_{x_\beta}S(\boldsymbol{U}_I, \boldsymbol{x}_I)] = 0. \tag{21}$$

The quadrature operator commutes with partial derivation with respect to x_β, so the last term above is equivalent to

$$\mathcal{Q}[\partial_{x_\beta}S(\boldsymbol{U}_I, \boldsymbol{x}_I)] = \partial_{x_\beta}\mathcal{Q}[S(\boldsymbol{U}_I, \boldsymbol{x}_I)]. \tag{22}$$

Similarly, the terms of the second summation in (21) can be rewritten as

$$\mathcal{Q}[\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{U}_I, \partial_{x_\beta}\boldsymbol{U}_I)] = \partial_{x_\alpha}\mathcal{Q}[\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{U}_I, \partial_{x_\beta}\boldsymbol{U}_I)] + \partial_{x_\beta}\mathcal{Q}[\frac{1}{2}\Omega^{(\alpha)}(\partial_{x_\alpha}\boldsymbol{U}_I, \boldsymbol{U}_I)]. \tag{23}$$

Finally, consider a term in the first sum in (21) and apply Lemma 1:

$$\begin{aligned}
\mathcal{Q}[\Omega^{(\alpha)}(\boldsymbol{U}_I^{x_\alpha}, \partial_{x_\beta}\boldsymbol{U}_I)] &= |\Delta\boldsymbol{x}|\sum_{I\in\mathbb{P}} b_I\Omega^{(\alpha)}(\boldsymbol{U}_I^{x_\alpha}, \partial_{x_\beta}\boldsymbol{U}_I)\\
&= |\Delta\boldsymbol{x}|\sum_{J\in\mathbb{Q}^\alpha}\sum_{j=1}^{s^\alpha} b_J b^\alpha_j\Omega^{(\alpha)}(\boldsymbol{U}^{x_\alpha}_{(J;j)}, \partial_{x_\beta}\boldsymbol{U}_{(J;j)})\\
&= |\Delta\boldsymbol{x}|\sum_{J\in\mathbb{Q}^\alpha} b_J\left\{\partial_{x_\beta}\left[\sum_{j=1}^{s^\alpha} b^\alpha_j\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{U}^{x_\alpha}_{(J;j)}, \boldsymbol{U}_{(J;j)})\right] + \frac{1}{\Delta x_\alpha}(F^{\alpha,1}_{\beta,J} - F^{\alpha,0}_{\beta,J})\right\}\\
&= \partial_{x_\beta}\mathcal{Q}[\frac{1}{2}\Omega^{(\alpha)}(\boldsymbol{U}_I^{x_\alpha}, \boldsymbol{U}_I)] + \frac{1}{\Delta x_\alpha}(F^{\alpha,1}_\beta - F^{\alpha,0}_\beta).
\end{aligned} \tag{24}$$

Substituting (22), (23) and (24) into (21) and using the definitions (18), (19) and (20) yields (17). □

Example. If we consider $d = 3$, $d^* = 2$, and let $\boldsymbol{x} = (x, y, t)$, then there are no continuous flux densities f^α, e is the energy density and $F^{1,j}$ and $F^{2,j}$, $j = 0, 1$, are the discrete energy flux densities in the x and y directions respectively. Equation (17) expresses the conservation of energy by the spatial semi-discretization

$$\partial_t e + \frac{1}{\Delta x}(F^{1,1} - F^{1,0}) + \frac{1}{\Delta y}(F^{2,1} - F^{2,0}) = 0.$$

This result has been noted for the specific example of the nonlinear Klein-Gordon equation in (Reich 2000*b*). Reich and co-workers have have found analogous results for other multisymplectic methods in (Reich 2000*a*, Bridges & Reich 2001, Moore & Reich 2003*a*, Moore & Reich 2003*b*). The above energy conservation law also holds when the multisymplectic Hamiltonian S depends explicitly on x and y.

Theorem 1 only gives conservation laws in the semi-discrete case. When $S(\boldsymbol{u})$ is quadratic (linear PDEs), fully discrete local conservation of energy and momentum are obtained. However, in the following section we obtain a fully discrete local conservation law of wave action, which is independent of the nonlinearity of the PDE.

3.3. Discrete conservation law of wave action

Consider a multisymplectic PDE (2) on a d^*-dimensional space-time, and define $d - d^*$ ensemble parameters $x_{d^*+1}, \ldots, x_d$, each 2π-periodic and associated to trivial presymplectic operators $J^{(\beta)} = 0$, $\beta = d^* + 1, \ldots, d$. Consider a full discretization on space-time (left continuous in the ensemble coordinates). In this case, the densities f^β are zero. Taking the loop integral of (17) with respect to each of the x_β, $\beta = d^* + 1, \ldots, d$, yields a discrete conservation law of wave action:

Corollary 1 *Let the coordinates x_β, $\beta = d^* + 1, \ldots, d$, be periodic with period 2π and associated to trivial presymplectic operators $J^{(\beta)} = 0$. Then for each $\beta = d^* + 1, \ldots, d$, the following discrete wave action conservation law holds*

$$\sum_{\alpha=1}^{d^*} \frac{1}{\Delta x_\alpha} (\mathcal{F}_\beta^{\alpha,1} - \mathcal{F}_\beta^{\alpha,0}) = 0, \qquad (25)$$

where

$$\mathcal{F}_\beta^{\alpha,j} = \oint F_\beta^{\alpha,j}\, dx_\beta, \quad j = 0, 1.$$

Note that the wave action conservation law holds for nonlinear problems, for problems (2) where S depends explicitly on the space-time coordinated $x_1, \ldots, x_d^*$ (where energy and momentum are not conserved), and for any tensor product grid (we have looked at a single grid cell here, without any reference to the size of neighboring cells). This discrete conservation law is the discrete analog of the general wave action conservation law of (Hayes 1970) and is an exact law, requiring no assumptions of near linearity of the solution or small amplitude perturbations. However, like the result of (Hayes 1970), the utility of this result depends on the identification of the ensemble parameters $x_{d^*+1}, \ldots x_d$.

4. Numerical illustration

As an illustration, let us consider the Korteweg-de Vries equation

$$u_t + (6u^2 + u_{xx})_x = 0.$$

This can be written in multisymplectic form (1) (Ascher & McLachlan 2004) with $\boldsymbol{u} = (u, v, w, \phi)^T$,

$$S(\boldsymbol{u}) = uw - 2u^3 - \frac{v^2}{2}$$

The matrices K and L have nonzero elements $K_{14} = -K_{41} = 1/2$ and $L_{12} = L_{34} = -L_{21} = -L_{43} = 1$.

The KdV equation has solitary wave solutions of the form (Whitham 1999)

$$u(t,x) = a\,\mathrm{sech}^2\left[(\frac{a}{2})^{1/2}(x-ct)\right] \tag{26}$$

where a is the amplitude, and the speed c is equal to $2a$.

Whitham considers a train of solitary waves with slowly varying amplitude $a = a(\epsilon x, \epsilon t)$. Assuming the train is periodic to lowest order approximation in ϵ, the wave action conservation law is obtained by averaging over the phase (Whitham 1999)

$$\partial_t(a^{3/2}) + \partial_x(\frac{6}{5}a^{5/2}) = 0. \tag{27}$$

This equation is the lowest order term in an asymptotic expansion of (6) in the parameter ϵ, and only holds approximately. In particular it is hyperbolic and its solution eventually develops a shock.

We discretized the KdV equation using the implicit midpoint rule ($s = 1$, $c_1 = a_{11} = 1/2$, $b_1 = 1$) in space and time, i.e. the multisymplectic Preissman/Keller box scheme (Bridges & Reich 2001), on the domain $[0, \ell)$ with periodic boundary conditions. The initial condition consisted of a superposition of 10 equally spaced solitary waves (26), with continously varying amplitude

$$a(x) = 1 + \epsilon \sin(2\pi x/\ell).$$

We took $\ell = 200$ and discretized on a grid with 1000 meshpoints. Time integration was carried out on $[0, 100]$ with stepsize 1/40.This discretization is actually rather coarse on the scale of a solitary wave.

The solution in space-time is shown at the top of Figure 1. Colors in the plot represent the amplitude of the solution. The solitary waves are initially equally spaced. Those with larger amplitude move faster and overtake the slower waves, at approximately time $t = 70$.

We also computed the solution to the action conservation law (27), using a central difference discretization. A contour plot of the amplitude $a(x,t)$ is shown in the bottom of Figure 1. The contour levels correspond to the initial amplitudes of the solitary waves in the KdV simulation. At approximately $t = 75$, as the solitary waves start to overtake each other, the action density forms a shock, and the solution becomes oscillatory. At this point the lowest order approximation is no longer sufficient. We note however that up to time $t = 70$, the action contours are in excellent agreement with the soliton peaks.

5. Concluding remarks

In this paper we have given the explicit form of the energy-momentum conservation law for multisymplectic Runge-Kutta semi-discretizations. This conservation law implies conservation of wave action over an arbitrary number of ensemble loop parameters in phase space, each associated to the trivial presymplectic operator, and the explicit form of these conservation laws has also been given here. A discrete wave action conservation law analogous to (25) also holds for the space-time generalization of the Störmer-Verlet method (Bridges & Reich 2001), also obtained by loop integration applied to a semi-discrete conservation law. Appealing to the Noether theory, one may expect that any method that can be derived from a variational principle (Marsden et al. 1998) will also conserve wave action, at least in a global sense.

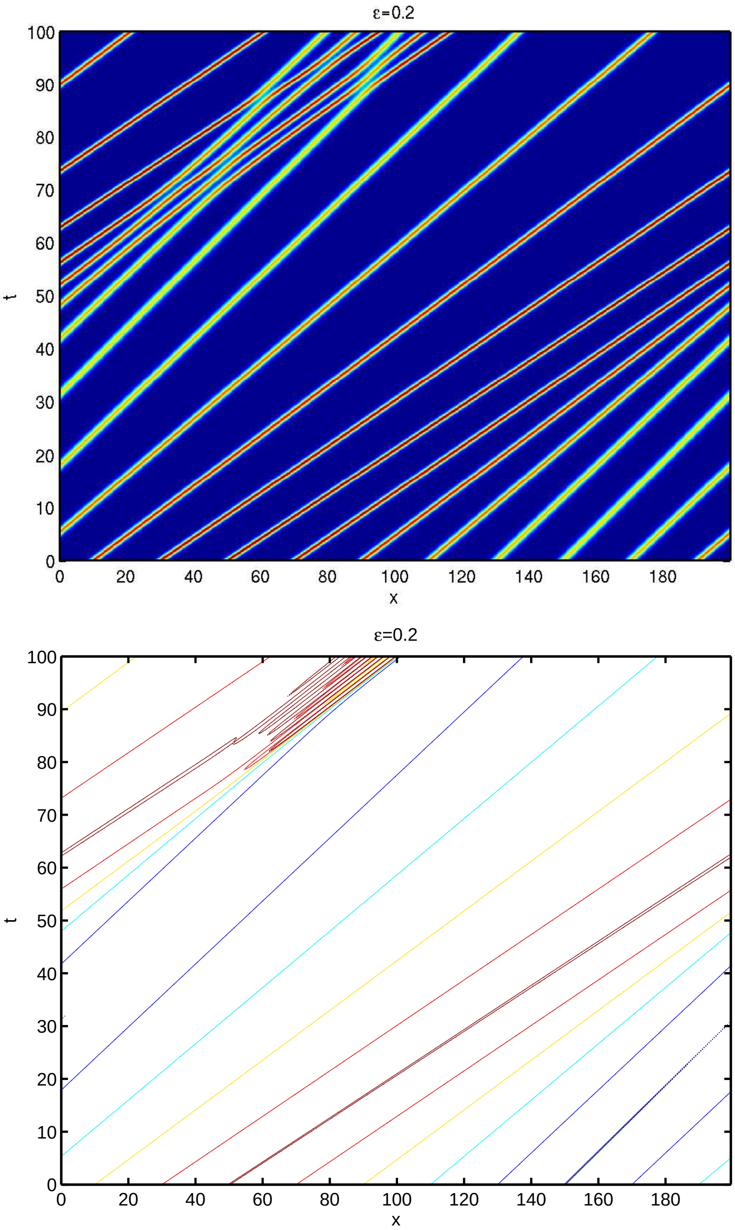

Figure 1. Comparison of multisymplectic box scheme solution (top) and level sets of action (bottom) for a train of KdV solitons.

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