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Conservation of wave action under multisymplectic discretizations

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ABSTRACT

In this paper we discuss the conservation of wave action under numerical discretization by variational and multisymplectic methods. Both the general wave action conservation defined with respect to a smooth, periodic, one-parameter ensemble of flow realizations and the specific wave action based on an approximated and averaged Lagrangian are addressed in the numerical context. It is found that the discrete variational formulation gives rise in a natural way not only to the discrete wave action conservation law but to a generalization of the numerical dispersion relation to the case of variable coefficients. Indeed a fully discrete analog of the modulation equations arises. On the other hand the multisymplectic framework gives easy access to the conservation law for the general class of multisymplectic Runge-Kutta methods. A numerical experiment confirms conservation of wave action to machine precision and suggests that the solution of the discrete modulation equations approximates the numerical solution to order $\mathcal{O}(\varepsilon)$ on intervals of $\mathcal{O}(\varepsilon^{-1})$.

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Conservation of wave action under multisymplectic discretizations

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Abstract. In this paper we discuss the conservation of wave action under numerical discretization by variational and multisymplectic methods. Both the general wave action conservation defined with respect to a smooth, periodic, one-parameter ensemble of flow realizations and the specific wave action based on an approximated and averaged Lagrangian are addressed in the numerical context. It is found that the discrete variational formulation gives rise in a natural way not only to the discrete wave action conservation law but to a generalization of the numerical dispersion relation to the case of variable coefficients. Indeed a fully discrete analog of the modulation equations arises. On the other hand the multisymplectic framework gives easy access to the conservation law for the general class of multisymplectic Runge-Kutta methods. A numerical experiment confirms conservation of wave action to machine precision and suggests that the solution of the discrete modulation equations approximates the numerical solution to order $\mathcal{O}(\varepsilon)$ on intervals of $\mathcal{O}(\varepsilon^{-1})$.

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1. Introduction

The wave action conservation law was introduced in (Whitham 1965) to study modulations of wave trains in slowly varying media. The approach follows by substituting a wave train with slowly varying amplitude, wave number and frequency into the variational principle, neglecting terms of higher order in a small perturbation parameter, and averaging the Lagrangian over phase to arrive at a variational principle for the modulation equations. Whitham's original theory thus leads to an approximate conservation law. A generalized form of the conservation law of wave action was introduced by (Hayes 1970), who considered a periodic, one-parameter family of solutions to the Euler-Lagrange equations. Conservation of wave action then follows from Noether's theorem, due to the trivial invariance of the action integral under translations in the ensemble parameter. This in turn makes Hayes's theory an exact one. The identification of Hayes's ensemble parameter with a phase shift relates the two theories (see (Hayes 1970) and (Grimshaw 1984) for more discussion). The concept of wave action conservation was further extended in (Whitham 1970), and a full treatment is given in the monograph (Whitham 1999).

The utility of the wave action 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. An important example is the case of waves defined on a slowly moving background flow, such as shallow water gravity waves on a slowly evolving potential vorticity field. The theory has therefore found application in wave-mean field interactions (Bretherton & Garrett 1969, Andrews & McIntyre 1978, Grimshaw 1984). Another important application is the instability theory of traveling waves (see (Bridges 1997*b*, Bridges 1997*a*) and the references therein). 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).

In this paper we consider wave equations in one space and one time dimension with a single wave action ensemble parameter. The results are easily generalized to higher dimensional space-time, however (Frank 2006). In §3 we will show that a number of multisymplectic numerical discretizations as developed in (Bridges & Reich 2001, Reich 2000*b*) satisfy a discrete conservation law of wave action in the sense of (Hayes 1970). This result is a corollary to the fact that multisymplectic semi-discretizations satisfy a semi-discrete energy-momentum conservation in each continuous (i.e. undiscretized) coordinate, which follows from the Noether theory for multisymplectic PDEs (Bridges 1997*b*). The latter has been shown for special cases in the literature (Reich 2000*b*), and a very general statement for the class of multisymplectic Runge-Kutta box schemes is treated in (Frank 2006). In §4 we prove wave action conservation for this class of methods in the current setting. Additionally we will consider in §3.1.1 a discrete variational integrator (Marsden et al. 1998, Marsden & West 2001) applied to the linear Klein-Gordon equation with slowly varying coefficients, for which a discrete averaged Lagrangian is obtained which yields discrete versions of the modulation equations. It is curious that the wave action conservation law so obtained is identical to the exact one obtained by ensemble averaging, i.e. no approximation is necessary in the discrete case. In other words Whitham's and Hayes's wave action concepts are equivalent in the discrete setting.

In §2 wave action conservation in the continuous case is reviewed, both in the Lagrangian and multisymplectic Hamiltonian settings. In §5 we conclude with a numerical computation of the linear Klein-Gordon equation with slowly varying coefficients.

To the best of our knowledge this is the first paper to study discrete conservation of wave action under numerical discretization. At this time, it is difficult to anticipate the significance of this property. One can say, however, that conservation of wave action is a property of certain solutions of continuous wave equations which is inherited under discretization by the variational and multisymplectic methods considered here, and as such it further attests to the realism of simulations by such methods.

2. Review of wave action conservation for continuous systems

2.1. Wave action conservation over a continuous ensemble

The concept of wave action conservation was developed in a variational setting. Consider a wave equation derivable from a variational principle with Lagrangian L

(Marsden & Ratiu 1994):

$$\mathcal{L} = \int L(u_t, u_x, u, t, x) dx dt. \quad (1)$$

The Euler-Lagrange equations are

$$\frac{\delta \mathcal{L}}{\delta u} = \partial_t \left(\frac{\partial L}{\partial u_t} \right) + \partial_x \left(\frac{\partial L}{\partial u_x} \right) - \frac{\partial L}{\partial u} = 0. \quad (2)$$

Due to the explicit dependence of L on time t and space x , solutions of the Euler-Lagrange equations will not conserve energy or momentum in general. Suppose, however, that (2) possesses an ensemble of solutions $u(t, x, \theta_0)$ that can be smoothly parameterized by a closed loop in phase space, with loop parameter θ_0 . The derivative of the Lagrangian with respect to this parameter is

$$\frac{dL}{d\theta_0} = \frac{\partial L}{\partial u_t} u_{t\theta_0} + \frac{\partial L}{\partial u_x} u_{x\theta_0} + \frac{\partial L}{\partial u} u_{\theta_0}.$$

Solving (2) for $\frac{\partial L}{\partial u}$ and substituting into the above expression gives

$$\frac{dL}{d\theta_0} = \partial_t \left(\frac{\partial L}{\partial u_t} u_{\theta_0} \right) + \partial_x \left(\frac{\partial L}{\partial u_x} u_{\theta_0} \right).$$

Integrating this relation around a loop in θ_0 yields the *conservation law of wave action*:

$$\partial_t \mathcal{A} + \partial_x \mathcal{B} = 0, \quad \mathcal{A} = \frac{1}{2\pi} \oint \frac{\partial L}{\partial u_t} u_{\theta_0} d\theta_0, \quad \mathcal{B} = \frac{1}{2\pi} \oint \frac{\partial L}{\partial u_x} u_{\theta_0} d\theta_0, \quad (3)$$

where \mathcal{A} is the wave action density and \mathcal{B} is the wave action flux.

2.1.1. Example: Klein-Gordon equation, averaged Lagrangian As a concrete example let us take the linear dispersive Klein-Gordon equation in a slowly varying medium:

$$u_{tt} = (\alpha(t, x)^2 u_x)_x - \beta(t, x)^2 u. \quad (4)$$

This equation was used in (Whitham 1970) to illustrate the above concepts. Equation (4) is the Euler-Lagrange equation associated to the action integral

$$\mathcal{L} = \int \frac{u_t^2}{2} - \alpha(t, x)^2 \frac{u_x^2}{2} - \beta(t, x)^2 \frac{u^2}{2} dx dt. \quad (5)$$

For this Lagrangian, the wave action density and flux (3) read

$$\mathcal{A} = \frac{1}{2\pi} \oint u_t u_{\theta_0} d\theta_0, \quad \mathcal{B} = \frac{1}{2\pi} \oint \alpha^2 u_x u_{\theta_0} d\theta_0, \quad (6)$$

In application of the theory to slow modulations of nearly periodic wave trains, we assume that α and β are slowly varying with respect to time and space, i.e. $\alpha = \alpha(T, X)$, $\beta = \beta(T, X)$, where $X = \varepsilon x$, $T = \varepsilon t$ for small parameter ε . We are interested in a family of nearly sinusoidal solutions with slowly varying amplitude, frequency, and wave number, parameterized by a phase shift. To that end we make the ansatz

$$u(t, x) = A(T, X) \sin(\theta(t, x) + \theta_0), \quad (7)$$

$$\theta(t, x) = \varepsilon^{-1} \Theta(T, X),$$

$$\theta_t(t, x) = -\omega(T, X), \quad (8)$$

$$\theta_x(t, x) = \kappa(T, X), \quad (9)$$

where θ_0 is a phase shift. For such a solution, the wave action density and flux (6) can be integrated to yield

$$\mathcal{A} = -\frac{1}{2}A^2\omega, \quad \mathcal{B} = \frac{1}{2}\alpha^2 A^2\kappa. \quad (10)$$

An alternative derivation proceeds by substituting (7) directly into the action integral (5) and averaging over θ_0 . The *averaged Lagrangian* is

$$\bar{L} = \frac{1}{2\pi} \oint L(u_t, u_x, u, t, x) d\theta_0 \quad (11)$$

$$= \frac{1}{2} \left[\frac{A^2\theta_t^2}{2} + \varepsilon^2 \frac{A_T^2}{2} \right] - \frac{1}{2}\alpha^2 \left[\frac{A^2\theta_x^2}{2} + \varepsilon^2 \frac{A_X^2}{2} \right] - \frac{1}{2}\beta^2 \frac{A^2}{2} \quad (12)$$

Neglecting terms of order ε^2 gives the action integral

$$\bar{\mathcal{L}} = \int \frac{1}{4} [A^2\theta_t^2 - \alpha^2 A^2\theta_x^2 - \beta^2 A^2] dx dt$$

in terms of A and θ . The Euler-Lagrange equations for this action principle are

$$\frac{\delta \bar{\mathcal{L}}}{\delta \theta} = \partial_t \left(\frac{1}{2} A^2 \theta_t \right) + \partial_x \left(\frac{1}{2} \alpha^2 A^2 \theta_x \right) = 0,$$

$$\frac{\delta \bar{\mathcal{L}}}{\delta A} = \theta_t^2 - \alpha^2 \theta_x^2 - \beta^2 = 0.$$

By making use of (8) and (9), one can express the above two equations in terms of the slowly varying quantities ω , κ and A :

$$\partial_t \left(-\frac{1}{2} A^2 \omega \right) + \partial_x \left(\frac{1}{2} \alpha^2 A^2 \kappa \right) = 0, \quad (13)$$

$$\omega^2 - \alpha^2 \kappa^2 - \beta^2 = 0, \quad (14)$$

$$\kappa_t + \omega_x = 0, \quad (15)$$

where the last of these is the compatibility condition $\theta_{xt} = \theta_{tx}$.

Equations (13)–(15) are the *modulation equations* which (approximately) govern the evolution of the envelope of the slowly varying wave train. The first of these is just the wave action conservation law (3) for the specific case (10). Equation (14) is a generalization of the dispersion relation to the case of variable coefficients.

It has been noted in (Whitham 1970) that although (3), (10) were obtained directly through an ensemble average over θ_0 , (13) was only obtained after neglecting terms of higher order in ε , and is therefore an approximate conservation law. We will refer to the former, exact conservation with respect to an ensemble of flow realizations as Hayes's wave action, and the latter, approximate conservation law as Whitham's wave action. This paper primarily deals with the former, although for specific examples we will always turn to the latter.

Note that, while (13) is derived by considering a family of solutions, in its final form it applies to the amplitude, frequency and wave number of an individual solution out of that family (it is local in the ensemble variable). This conservation law holds even when the Lagrangian (1) depends explicitly on t and x , i.e. when energy and momentum are not conserved.

2.2. Multisymplectic structure and wave action

By taking a complete Legendre transformation of (1) not only with respect to u_t but also with respect to u_x , one may derive a Hamiltonian wave equation in the abstract multisymplectic form (Bridges 1997b)

$$J\mathbf{u}_t + K\mathbf{u}_x = \nabla S(\mathbf{u}, t, x), \quad (16)$$

where $\mathbf{u}(t, x) \in \mathbf{R}^N$, $J^T = -J$ and $K^T = -K$ are $N \times N$ skew-symmetric matrices, and $S : \mathbf{R}^N \times \mathbf{R} \times \mathbf{R} \rightarrow \mathbf{R}$ is a functional which may depend on t and x . The papers (Bridges 1997a) and (Bridges 1997b) provide a complete and accessible introduction to multisymplectic structure and some of its applications.

Suppose S has no explicit dependence on t in (16). Then taking the vector inner product of (16) with \mathbf{u}_t gives

$$\mathbf{u}_t^T J\mathbf{u}_t + \mathbf{u}_t^T K\mathbf{u}_x = \mathbf{u}_t^T \nabla S(\mathbf{u}, x). \quad (17)$$

The first term is zero by skew-symmetry of J . Using the identity

$$\mathbf{u}_t^T K\mathbf{u}_x = \partial_t \left(\frac{1}{2} \mathbf{u}^T K\mathbf{u}_x \right) + \partial_x \left(\frac{1}{2} \mathbf{u}_t^T K\mathbf{u} \right), \quad (18)$$

and the fact that the right side of (17) is just the total derivative of S with respect to t , the conservation law

$$e_t + f_x = 0, \quad e = \frac{1}{2} \mathbf{u}^T K\mathbf{u}_x - S, \quad f = \frac{1}{2} \mathbf{u}_t^T K\mathbf{u} \quad (19)$$

is obtained. In (Bridges 1997b) it is observed that this is the energy conservation law associated with the invariance of (16) to time translations. If S does not depend explicitly on x , the associated momentum conservation law follows analogously by taking the inner product of (16) with \mathbf{u}_x .

The wave action conservation principle of (Hayes 1970) has been cast in multisymplectic form in (Bridges 1997a). The idea is to consider a one-parameter ensemble of solutions $\mathbf{u}(t, x, \theta_0)$ to (16) smoothly parameterized by a closed loop in phase space $\theta_0 \in \mathcal{S}^1$. Taking the vector inner product of (16) with \mathbf{u}_{θ_0} and using the same reasoning as above yields the conservation law

$$\partial_{\theta_0} \left(\frac{1}{2} \mathbf{u}^T J\mathbf{u}_t + \frac{1}{2} \mathbf{u}^T K\mathbf{u}_x - S \right) + \partial_t \left(\frac{1}{2} \mathbf{u}_{\theta_0}^T J\mathbf{u} \right) + \partial_x \left(\frac{1}{2} \mathbf{u}_{\theta_0}^T K\mathbf{u} \right) = 0. \quad (20)$$

The ensemble average gives Hayes's conservation law of wave action

$$\partial_t \mathcal{A} + \partial_x \mathcal{B} = 0, \quad \mathcal{A} = \frac{1}{4\pi} \oint \mathbf{u}_{\theta_0}^T J\mathbf{u} d\theta_0, \quad \mathcal{B} = \frac{1}{4\pi} \oint \mathbf{u}_{\theta_0}^T K\mathbf{u} d\theta_0. \quad (21)$$

2.2.1. Example: multisymplectic description of the Klein-Gordon equation The Klein-Gordon equation can be cast in the form (16) by introducing the Legendre transformations $v := \partial L / \partial u_t = u_t$ and $w := \partial L / \partial u_x = -\alpha^2 u_x$. Then one finds, with $\mathbf{u} = (u, v, w)$, that $S = \frac{1}{2}(v^2 - \alpha^{-2}w^2 + \beta^2 u^2)$ and

$$J = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

The conservation law (21) holds with

$$\mathcal{A} = \frac{1}{4\pi} \oint v_{\theta_0} u - u_{\theta_0} v d\theta_0 = -\frac{1}{2\pi} \oint u_{\theta_0} u_t d\theta_0$$

and

$$\mathcal{B} = \frac{1}{4\pi} \oint w_{\theta_0} u - u_{\theta_0} w \, d\theta_0 = \frac{1}{2\pi} \oint \alpha^2 u_{\theta_0} u_x \, d\theta_0,$$

which are precisely (6).

The extension of this theory to higher dimensional space-time is straightforward. Additional dimensions may be included within the multisymplectic framework with an additional term $K^{(d)} \mathbf{u}_{x_d}$ ($K^{(d)}$ skew-symmetric) for each additional coordinate x_d . If S is independent of x_d , then a momentum equation analogous to (19) may be found by taking the inner product of (16) with \mathbf{u}_{x_d} and applying the identity (18). Indeed, the wave action conservation law (20) can also be derived in this way by considering $x_0 \equiv \theta_0$ as an additional spatial dimension with periodic boundary conditions, with associated trivial skew-symmetric matrix $K^0 = 0$. Then it is the translation symmetry in θ_0 which leads to (20). For a general statement in the context of multisymplectic Runge-Kutta discretizations, see (Frank 2006).

In (Bridges 1997a) it is shown that (21) is equivalent via Stokes theorem to a local conservation law of symplecticity. The defining property of a multisymplectic numerical discretization is that it satisfies a discrete version of the local conservation law of symplecticity. However, since Stokes theorem does not in general hold after discretization, it is not immediate that multisymplectic discretizations have an analogous wave action conservation law. In the next section we identify such conservation laws for some discrete variational and multisymplectic methods.

3. Discrete wave action conservation

3.1. Wave action conservation for a discrete variational integrator

Below we follow a derivation analogous to that of §2.1 for a discrete variational integrator, see (Marsden et al. 1998, Marsden & West 2001). Define a discrete Lagrangian by

$$L_i^n := L\left(\frac{u_i^{n+1} - u_i^n}{\Delta t}, \frac{u_{i+1}^n - u_i^n}{\Delta x}, u_i^n, x_i, t_n\right). \quad (22)$$

The discrete action integral (up to boundary conditions) is

$$\mathcal{L}_D = \sum_{i,n} L_i^n,$$

and the discrete Euler-Lagrange equations are given by

$$0 = \frac{\partial \mathcal{L}_D}{\partial u_i^n} = \frac{1}{\Delta t} (L_{1_i}^n - L_{1_i}^{n-1}) + \frac{1}{\Delta x} (L_{2_i}^n - L_{2_{i-1}}^n) - L_{3_i}^n, \quad (23)$$

where $L_{p_i}^n$ denotes the partial derivative of L with respect to its p th argument, evaluated at the same indices as (22). The scheme (23) will be referred to as the discrete variational Euler scheme.

Next we assume a family of discrete functions $u_i^n(\theta_0)$, satisfying (23) and smooth and periodic in θ_0 . We compute the derivative of L_i^n with respect to θ_0 :

$$\frac{\partial L_i^n}{\partial \theta_0} = L_{1_i}^n \partial_{\theta_0} \frac{u_i^{n+1} - u_i^n}{\Delta t} + L_{2_i}^n \partial_{\theta_0} \frac{u_{i+1}^n - u_i^n}{\Delta x} + L_{3_i}^n \partial_{\theta_0} u_i^n.$$

Substituting (23) into the last term on the right and rearranging gives

$$\frac{\partial L_i^n}{\partial \theta_0} = \frac{1}{\Delta t} (L_{1_i}^n \partial_{\theta_0} u_i^{n+1} - L_{1_i}^{n-1} \partial_{\theta_0} u_i^n) + \frac{1}{\Delta x} (L_{2_i}^n \partial_{\theta_0} u_{i+1}^n - L_{2_{i-1}}^n \partial_{\theta_0} u_i^n).$$

Finally, taking the ensemble average yields a discrete conservation law. That is,

Proposition 1 *The discrete variational Euler scheme (23) satisfies the discrete conservation law of wave action*

$$\frac{1}{\Delta t}(\mathcal{A}_i^{n+1/2} - \mathcal{A}_i^{n-1/2}) + \frac{1}{\Delta x}(\mathcal{B}_{i+1/2}^n - \mathcal{B}_{i-1/2}^n) = 0, \quad (24)$$

where

$$\mathcal{A}_i^{n+1/2} = \frac{1}{2\pi} \oint L_{1i}^n \partial_{\theta_0} u_i^{n+1} d\theta_0, \quad \mathcal{B}_{i+1/2}^n = \frac{1}{2\pi} \oint L_{2i}^n \partial_{\theta_0} u_{i+1}^n d\theta_0. \quad (25)$$

Equation (24) is the discrete analog of (3).

3.1.1. Example: variational discretization of the Klein-Gordon equation Now let us consider a variational integrator for (4). The action principle (5) is approximated by the sum

$$\mathcal{L} = \sum_{i,n} \frac{1}{2} \left(\frac{u_i^{n+1} - u_i^n}{\Delta t} \right)^2 - (\alpha_{i+1/2}^n)^2 \frac{1}{2} \left(\frac{u_{i+1}^n - u_i^n}{\Delta x} \right)^2 - (\beta_i^n)^2 \frac{1}{2} (u_i^n)^2. \quad (26)$$

As in the continuous case, let us assume a family of discrete, slowly modulated waves of the form

$$u_i^n = A_i^n \sin(\theta_i^n + \theta_0). \quad (27)$$

Substituting this family directly into (24) and taking the ensemble average yields the discrete wave action density

$$\mathcal{A}_i^{n+1/2} = \frac{1}{2} A_i^n A_i^{n+1} \Delta t^{-1} \sin(\theta_i^{n+1} - \theta_i^n) \quad (28)$$

and discrete flux

$$\mathcal{B}_{i+1/2}^n = \frac{1}{2} (\alpha_{i+1/2}^n)^2 A_i^n A_{i+1}^n \Delta x^{-1} \sin(\theta_{i+1}^n - \theta_i^n). \quad (29)$$

These quantities are second order approximations to (10).

It is also instructive to follow the averaged Lagrangian approach used in §2.1.1. Substituting (27) into (26) and averaging over θ_0 gives the averaged variational principle

$$\begin{aligned} \bar{\mathcal{L}} = \sum_{i,n} \frac{1}{4\Delta t^2} & [(A_i^{n+1})^2 - 2A_i^n A_i^{n+1} \cos(\theta_i^{n+1} - \theta_i^n) + (A_i^n)^2] \\ & + \frac{(\alpha_{i+1/2}^n)^2}{4\Delta x^2} [(A_{i+1}^n)^2 - 2A_i^n A_{i+1}^n \cos(\theta_{i+1}^n - \theta_i^n) + (A_i^n)^2] \\ & + \frac{(\beta_i^n)^2}{4} (A_i^n)^2. \end{aligned} \quad (30)$$

Taking the discrete variation with respect to θ_i^n produces precisely (24) with (28) and (29):

$$\begin{aligned} 0 = \frac{1}{2\Delta t^2} & [A_i^{n+1} A_i^n \sin(\theta_i^{n+1} - \theta_i^n) - A_i^n A_i^{n-1} \sin(\theta_i^n - \theta_i^{n-1})] + \\ & \frac{1}{2\Delta x^2} [(A_{i+1}^n)^2 A_i^n A_{i+1}^n \sin(\theta_{i+1}^n - \theta_i^n) - (\alpha_{i-1/2}^n)^2 A_i^n A_{i-1}^n \sin(\theta_i^n - \theta_{i-1}^n)] \end{aligned} \quad (31)$$

In contrast to the continuous case, it is unnecessary to neglect any small terms in the Lagrangian to obtain the identical formulation. Hayes's ensemble average over

phase shift and Whitham's averaged Lagrangian give formally identical wave action conservation laws, without neglecting any higher order terms in the Lagrangian.

The variation of (30) with respect to A_i^n gives a generalized numerical dispersion relation for variable coefficients:

$$0 = \frac{1}{\Delta t^2} \left[A_i^n - \frac{1}{2} A_i^{n+1} \cos(\theta_i^{n+1} - \theta_i^n) - \frac{1}{2} A_i^{n-1} \cos(\theta_i^n - \theta_i^{n-1}) \right] + \frac{1}{\Delta x^2} \left[\frac{(\alpha_{i+1/2}^n)^2 + (\alpha_{i-1/2}^n)^2}{2} A_i^n - (\alpha_{i+1/2}^n)^2 \frac{1}{2} A_{i+1}^n \cos(\theta_{i+1}^n - \theta_i^n) - (\alpha_{i-1/2}^n)^2 \frac{1}{2} A_{i-1}^n \cos(\theta_i^n - \theta_{i-1}^n) \right] + \frac{(\beta_i^n)^2}{2} A_i^n. \quad (32)$$

A discrete analog of the modulation equations (13)–(15) can be obtained by eliminating θ_i^n through the substitutions

$$\theta_i^{n+1} - \theta_i^n \equiv -\omega_i^{n+1/2} \Delta t, \quad \theta_{i+1}^n - \theta_i^n \equiv \kappa_{i+1/2}^n \Delta x$$

in (31) and (32). We then need the compatibility condition

$$\frac{1}{\Delta t} (\kappa_{i+1/2}^{n+1} - \kappa_{i+1/2}^n) + \frac{1}{\Delta x} (\omega_{i+1}^{n+1/2} - \omega_i^{n+1/2}) = 0. \quad (33)$$

Since the variables A_i^n , $\kappa_{i+1/2}^n$ and $\omega_i^{n+1/2}$ are all slowly varying, the discrete modulation equations could conceivably be solved on a coarser grid.

3.2. Discrete multisymplectic integrators

The wave action conservation law (31) may also be derived directly from a multisymplectic description. Consider a wave equation of the form (16).

Defining matrices J^+ , J^- , K^+ , K^- , to be the upper triangular and lower triangular parts of J and K , respectively, the *multisymplectic Euler* discretization of (16) is given by (Moore & Reich 2003a):

$$J^+ \frac{\mathbf{u}_i^{n+1} - \mathbf{u}_i^n}{\Delta t} + J^- \frac{\mathbf{u}_i^n - \mathbf{u}_i^{n-1}}{\Delta t} + K^+ \frac{\mathbf{u}_{i+1}^n - \mathbf{u}_i^n}{\Delta x} + K^- \frac{\mathbf{u}_i^n - \mathbf{u}_{i-1}^n}{\Delta x} = \nabla S(\mathbf{u}_i^n, x_i, t_n). \quad (34)$$

Next assume a family of numerical solutions, smoothly and periodically dependent on the parameter θ_0 , and compute the vector inner product of (34) with $\partial_{\theta_0} \mathbf{u}_i^n$. Rearranging, and using the fact that $(J^+)^T = -J^-$, $(K^+)^T = -K^-$ gives the semi-discrete conservation law[‡]

$$\begin{aligned} \partial_{\theta_0} \left[\frac{(\mathbf{u}_i^{n-1})^T J^+ \mathbf{u}_i^n - (\mathbf{u}_i^n)^T J^+ \mathbf{u}_i^n}{\Delta t} + \frac{(\mathbf{u}_{i-1}^n)^T K^+ \mathbf{u}_i^n - (\mathbf{u}_i^n)^T K^+ \mathbf{u}_i^n}{\Delta x} - S(\mathbf{u}_i^n, x_i, t_n) \right] \\ + \frac{(\partial_{\theta_0} \mathbf{u}_i^n)^T J^+ \mathbf{u}_i^{n+1} - (\partial_{\theta_0} \mathbf{u}_i^{n-1})^T J^+ \mathbf{u}_i^n}{\Delta t} + \frac{(\partial_{\theta_0} \mathbf{u}_i^n)^T K^+ \mathbf{u}_{i+1}^n - (\partial_{\theta_0} \mathbf{u}_{i-1}^n)^T K^+ \mathbf{u}_i^n}{\Delta x} \\ = 0. \end{aligned}$$

Integrating around a closed loop in θ_0 , the first term disappears, leaving a discrete conservation law of the form (24), i.e.

[‡] This expression also suggests the form of semi-discrete energy-momentum conservation laws for semi-discretizations with the multisymplectic Euler scheme.

Proposition 2 *The multisymplectic Euler scheme (34) satisfies the discrete wave action conservation law (24) with*

$$\mathcal{A}_i^{n+1/2} = \oint (\partial_{\theta_0} \mathbf{u}_i^n)^T J^+ \mathbf{u}_i^{n+1} d\theta_0, \quad \mathcal{B}_{i+1/2}^n = \oint (\partial_{\theta_0} \mathbf{u}_i^n)^T K^+ \mathbf{u}_{i+1}^n d\theta_0. \quad (35)$$

Since the above discretization is equivalent to the discrete Euler-Lagrange equations (23), these discrete density and flux functions are equal to (25). A larger class of multisymplectic discretizations will be dealt with in the next section.

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

In this section we derive discrete wave action conservation laws for a popular class of multisymplectic methods, the Runge-Kutta box schemes (Reich 2000b). It is sufficient to consider a single space-time grid cell $[t_0, t_1] \times [x_0, x_1]$.

The discretization is a composition of an s -stage Runge-Kutta method in time and an \tilde{s} -stage method in space, and the method coefficients (Hairer et al. 1993) are denoted analogously

$$c_m, b_m, a_{m\ell}, \quad m, \ell = 1, \dots, s \quad (36)$$

$$\tilde{c}_j, \tilde{b}_j, \tilde{a}_{jk}, \quad j, k = 1, \dots, \tilde{s} \quad (37)$$

The points (τ_m, ξ_j) , where $\tau_m = t_0 + c_m \Delta t$ and $\xi_j = x_0 + \tilde{c}_j \Delta x$, are collocation points.

With these definitions, the Runge-Kutta box scheme semi-discretization is defined by a set of $s \times \tilde{s}$ collocation equations

$$J \mathbf{T}_j^m + K \mathbf{X}_j^m = \nabla S(\mathbf{U}_j^m, \tau_m, \xi_j), \quad \begin{cases} j = 1, \dots, \tilde{s}, \\ m = 1, \dots, s, \end{cases} \quad (38)$$

where \mathbf{U}_j^m , \mathbf{T}_j^m and \mathbf{X}_j^m are stage vectors approximating, respectively, \mathbf{u} , \mathbf{u}_t and \mathbf{u}_x at (τ_m, ξ_j) . Additionally we have the relations

$$\begin{cases} \mathbf{U}_j^m = \mathbf{u}_j^0 + \Delta t \sum_{\ell=1}^s a_{m\ell} \mathbf{T}_j^\ell, \\ \mathbf{U}_j^m = \mathbf{u}_0^m + \Delta x \sum_{k=1}^{\tilde{s}} \tilde{a}_{jk} \mathbf{X}_k^m, \end{cases} \quad \begin{cases} j = 1, \dots, \tilde{s}, \\ m = 1, \dots, s. \end{cases} \quad (39)$$

In (39) the quantities \mathbf{u}_j^0 and \mathbf{u}_0^m approximate \mathbf{u} on the cell faces at (t_0, ξ_j) and (τ_m, x_0) , respectively. The values on the opposite faces are denoted \mathbf{u}_j^1 and \mathbf{u}_1^m and are obtained from

$$\begin{cases} \mathbf{u}_j^1 = \mathbf{u}_j^0 + \Delta t \sum_{m=1}^s b_m \mathbf{T}_j^m, \\ \mathbf{u}_1^m = \mathbf{u}_0^m + \Delta x \sum_{j=1}^{\tilde{s}} \tilde{b}_j \mathbf{X}_j^m, \end{cases} \quad \begin{cases} j = 1, \dots, \tilde{s}, \\ m = 1, \dots, s. \end{cases} \quad (40)$$

Additional formulas are necessary to relate the above quantities to gridpoint values (Frank et al. 2006). However, the relations (38), (39) and (40) 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 both coefficient sets $\{c_m, b_m, a_{m\ell}\}$ and $\{\tilde{c}_j, \tilde{b}_j, \tilde{a}_{jk}\}$ define symplectic RK methods (Hairer et al. 2002), i.e.

$$\begin{cases} b_m b_\ell - b_\ell a_{\ell m} - b_m a_{m\ell} = 0, & \forall m, \ell, \\ \tilde{b}_j \tilde{b}_k - \tilde{b}_k \tilde{a}_{kj} - \tilde{b}_j \tilde{a}_{jk} = 0, & \forall j, k. \end{cases} \quad (41)$$

The following lemma is the discrete analog of (18).

Lemma 1 Consider a skew-symmetric matrix $K \in \mathbf{R}^{N \times N}$ and a set of vectors $\mathbf{u}_0(\theta_0)$, $\mathbf{u}_1(\theta_0)$, $\mathbf{U}_j(\theta_0)$, $\mathbf{X}_j(\theta_0) \in \mathbf{R}^N$, $j = 1, \dots, \bar{s}$, smoothly dependent on a parameter θ_0 and satisfying the Runge-Kutta formulas

$$\mathbf{U}_j = \mathbf{u}_0 + \Delta k \sum_{k=1}^{\bar{s}} \tilde{a}_{jk} \mathbf{X}_k, \quad m = 1, \dots, s \quad (42)$$

$$\mathbf{u}_1 = \mathbf{u}_0 + \Delta k \sum_{j=1}^{\bar{s}} \tilde{b}_m \mathbf{X}_j. \quad (43)$$

For symplectic Runge-Kutta methods (41) the following identity holds:

$$\sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{U}_j^T K \mathbf{X}_j = \partial_{\theta_0} \left[\sum_{j=1}^{\bar{s}} \tilde{b}_j \frac{1}{2} \mathbf{U}_j^T K \mathbf{X}_j \right] + \frac{1}{\Delta x} (F_1 - F_0), \quad (44)$$

with $F_i = \frac{1}{2} \partial_{\theta_0} \mathbf{u}_i^T K \mathbf{u}_i$, $i = 0, 1$.

Proof. Substitute (43) into the definition of F^1 to obtain

$$\begin{aligned} \partial_{\theta_0} \mathbf{u}_1^T K \mathbf{u}_1 &= \partial_{\theta_0} \mathbf{u}_0^T K \mathbf{u}_0 + \Delta x \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{u}_0^T K \mathbf{X}_j + \Delta x \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{u}_0 \\ &\quad + \Delta x^2 \sum_{j,k=1}^{\bar{s}} \tilde{b}_j \tilde{b}_k \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{X}_k. \end{aligned} \quad (45)$$

Solving (42) for \mathbf{u}_0 , differentiating with respect to θ_0 , and substituting into the first series above yields

$$\begin{aligned} \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{u}_0^T K \mathbf{X}_j &= \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{U}_j^T K \mathbf{X}_j - \Delta x \sum_{j,k=1}^{\bar{s}} \tilde{b}_j \tilde{a}_{jk} \partial_{\theta_0} \mathbf{X}_k^T K \mathbf{X}_j \\ &= \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{U}_j^T K \mathbf{X}_j - \Delta x \sum_{j,k=1}^{\bar{s}} \tilde{b}_k \tilde{a}_{kj} \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{X}_k, \end{aligned}$$

where the skew-symmetry of K been used. Similarly, the second series becomes

$$\sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{u}_0 = \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{U}_j - \Delta x \sum_{j=1}^{\bar{s}} \tilde{b}_j \tilde{a}_{jk} \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{X}_k.$$

Substituting the above two formulas into (45) gives

$$\begin{aligned} \partial_{\theta_0} \mathbf{u}_1^T K \mathbf{u}_1 &= \partial_{\theta_0} \mathbf{u}_0^T K \mathbf{u}_0 + \Delta x \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{U}_j^T K \mathbf{X}_j + \Delta x \sum_{j=1}^{\bar{s}} \tilde{b}_j \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{U}_j \\ &\quad + \Delta x^2 \sum_{j,k=1}^{\bar{s}} (\tilde{b}_j \tilde{b}_k - \tilde{b}_k \tilde{a}_{kj} - \tilde{b}_j \tilde{a}_{jk}) \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{X}_k. \end{aligned} \quad (46)$$

For symplectic RK methods (41), the last term in (46) cancels. Finally we note that

$$\partial_{\theta_0} \mathbf{U}_j^T K \mathbf{X}_j + \partial_{\theta_0} \mathbf{X}_j^T K \mathbf{U}_j = 2 \partial_{\theta_0} \mathbf{U}_j^T K \mathbf{X}_j - \partial_{\theta_0} (\mathbf{U}_j^T K \mathbf{X}_j),$$

and (44) follows. \square

Next, by premultiplying (38) by $\partial_{\theta_0} \mathbf{U}_j^m$ and applying the quadrature over j and m ,

$$\sum_{j,m} b_m \tilde{b}_j (\partial_{\theta_0} \mathbf{U}_j^m)^T [J \mathbf{T}_j^m + K \mathbf{X}_j^m - \nabla S(\mathbf{U}_j^m, \tau_m, \xi_j)] = 0,$$

and applying Lemma 1, we arrive at the semi-discrete conservation law

$$\begin{aligned} \partial_{\theta_0} \sum_{j,m} b_m \tilde{b}_j \left[\frac{1}{2} (\mathbf{U}_j^m)^T J \mathbf{T}_j^m + \frac{1}{2} (\mathbf{U}_j^m)^T K \mathbf{X}_j^m - S(\mathbf{U}_j^m, \tau_m, \xi_j) \right] \\ + \frac{1}{\Delta t} (A^1 - A^0) + \frac{1}{\Delta x} (B_1 - B_0) = 0, \end{aligned} \quad (47)$$

where

$$\begin{aligned} A^n &= \sum_{j=1}^{\tilde{s}} \tilde{b}_j \frac{1}{2} (\partial_{\theta_0} \mathbf{u}_j^n)^T J \mathbf{u}_j^n, & n = 0, 1, \\ B_i &= \sum_{m=1}^s b_m \frac{1}{2} (\partial_{\theta_0} \mathbf{u}_i^m)^T K \mathbf{u}_i^m & i = 0, 1. \end{aligned}$$

Finally, taking the ensemble average of (47) around a loop in θ_0 proves

Proposition 3 *The multisymplectic Runge-Kutta discretization (38)–(41) satisfies the following discrete conservation law of wave action*

$$\frac{1}{\Delta t} (\mathcal{A}^1 - \mathcal{A}^0) + \frac{1}{\Delta x} (\mathcal{B}_1 - \mathcal{B}_0) = 0, \quad (48)$$

where

$$\begin{aligned} \mathcal{A}^n &= \frac{1}{2\pi} \oint \sum_{j=1}^{\tilde{s}} \tilde{b}_j \frac{1}{2} (\partial_{\theta_0} \mathbf{u}_j^n)^T J \mathbf{u}_j^n d\theta_0, & n = 0, 1, \\ \mathcal{B}_i &= \frac{1}{2\pi} \oint \sum_{m=1}^s b_m \frac{1}{2} (\partial_{\theta_0} \mathbf{u}_i^m)^T K \mathbf{u}_i^m d\theta_0, & i = 0, 1. \end{aligned}$$

Note that the discrete wave action conservation law (48) holds for nonlinear problems, for problems (16) where S depends explicitly on the space-time coordinated x and t (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. However, like the result of (Hayes 1970), the utility of this result depends on the identification of the ensemble parameter θ_0 .

Remark. By identifying θ_0 with another coordinate direction, say y , which need not be periodic, the semi-discrete conservation law (47) corresponds to the conservation of momentum associated with translation symmetry in the y dimension (since S exhibits no explicit dependence on y). As such, (47) is a more general statement of a semi-discrete conservation law of semi-discretizations, with respect to the momentum in the nondiscretized directions (Frank 2006). This semi-discrete conservation law has been noted in other contexts before, see (Reich 2000b, Reich 2000a, Bridges & Reich 2001, Moore & Reich 2003a, Moore & Reich 2003b, Hong & Li 2006).

5. Numerical experiment

In this section we illustrate discrete wave action conservation using the discrete variational/multisymplectic Euler method (23),(34), applied to a slowly modulated wave train solution of the Klein-Gordon equation (4). The domain is the interval $x \in [0, L)$ with $L = 2\pi/\varepsilon$ and periodic boundary conditions. The coefficients α and β are chosen to be

$$\alpha = 1 + \frac{1}{5} \sin\left(\frac{\pi}{27}\varepsilon t\right) \exp\left[-25\left(\frac{x}{L} - \frac{1}{2}\right)^2\right], \quad \beta = 1 - \cos\left(\frac{\pi}{20}\varepsilon t\right) \exp\left[-25\left(\frac{x}{L} - \frac{1}{2}\right)^2\right].$$

We take as initial condition a uniform, right-traveling wave train

$$u(0, x) = \sin(\kappa x + \theta_0), \quad v(0, x) = u_t(0, x) = -\omega \cos(\kappa x + \theta_0), \quad \kappa = \omega = \frac{4\pi}{\varepsilon L}.$$

For the discretization, we have $N = 30/\varepsilon$, $\Delta t = \varepsilon L/N$, and integrate to time $160/\varepsilon$.

For a linear problem, it is possible, by taking the derivative of (34) with respect to θ_0 , to also integrate numerically and determine u_{θ_0} and v_{θ_0} , using initial conditions

$$u_{\theta_0}(0, x) = \cos(\kappa x + \theta_0), \quad v_{\theta_0}(0, x) = \omega \sin(\kappa x + \theta_0).$$

Then, under the assumption that $u_i^n = \tilde{A}_i^n \sin(\tilde{\theta}_i^n + \theta_0)$, $\partial_{\theta_0} u_i^n = \tilde{A}_i^n \cos(\tilde{\theta}_i^n + \theta_0)$, we can approximate the amplitude and phase of the numerical solution by

$$\tilde{A}_i^n = \sqrt{(u_i^n)^2 + (\partial_{\theta_0} u_i^n)^2}, \quad \tilde{\theta}_i^n = \tan^{-1} \frac{u_i^n}{\partial_{\theta_0} u_i^n}. \quad (49)$$

Alternatively, we can integrate the discrete modulation equations (31), (32) to approximate A_i^n and θ_i^n . A comparison of the numerical solution and the amplitude obtained by a separate integration of (31), (32) is shown in Figure 1.

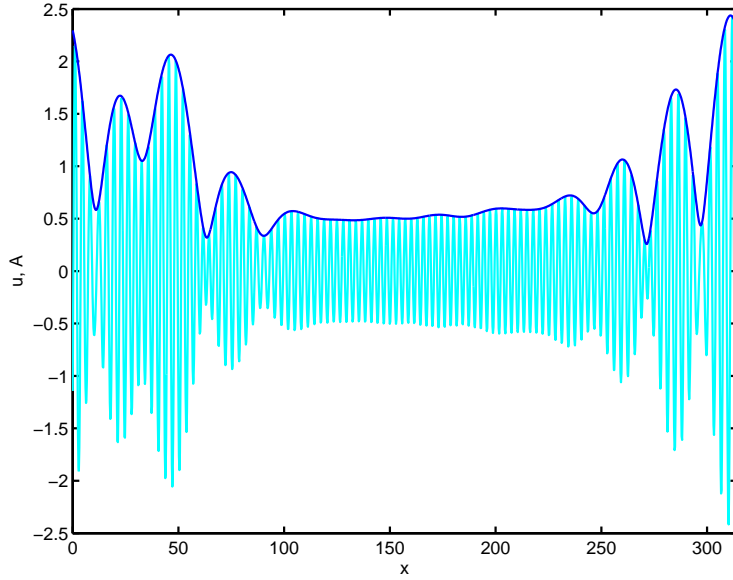


Figure 1. Solution u_i^n (light blue) and amplitude A_i^n (blue) at time $T = 160/\varepsilon$ for $\varepsilon = 0.02$.

The wave action density is given by (28). The total wave action at time t_n is given by

$$\mathcal{A}^n = \sum_i \mathcal{A}_i^n \Delta x.$$

This quantity is conserved to machine precision, as can be seen by applying the summation above to (31) with periodic boundary conditions. If we substitute \tilde{A}_i^n and $\tilde{\theta}_i^n$ as determined from (49) into (31), the residual is nonzero. Nonetheless, the total wave action is conserved in this case as well. Figure 2 compares the relative variation in total wave action to that of total energy for $\varepsilon = 0.05$. The total wave action is $2\pi/\varepsilon$ and the initial energy is $13.3/\varepsilon$.

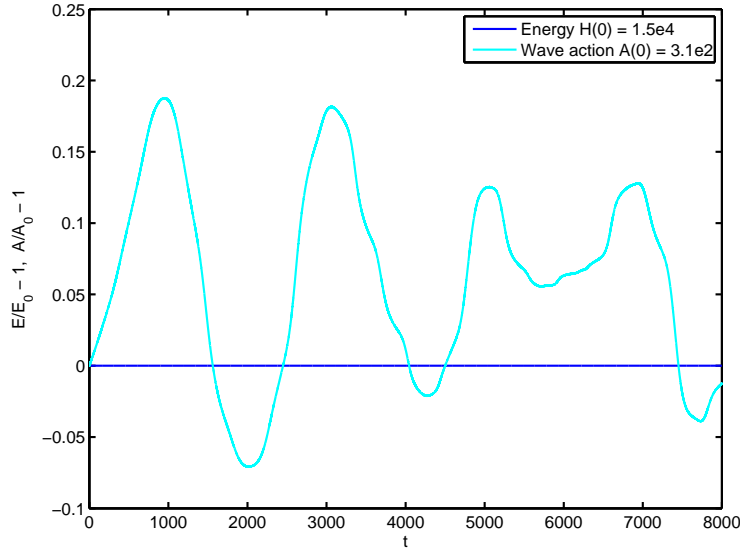


Figure 2. Relative variation in total energy (light blue) and total wave action (cyan) as a percentage of the initial value. $\varepsilon = 0.02$.

As a measure of the accuracy of the discrete modulation equations, we can measure the approximation error in the L_∞ -norm

$$e^n = \max_i |u_i^n - A_i^n \sin \theta_i^n|,$$

where again A_i^n and θ_i^n are obtained from a separate integration of (31), (32). This quantity is plotted as a function of time in Figure 3 for $\varepsilon = 0.4, 0.2, 0.1$ and 0.05 . The results are scaled in time to fit on one plot. The similarity of the error evolution suggests that the discrete modulation equations approximate the numerical solution to order $\mathcal{O}(\varepsilon)$ for intervals of $\mathcal{O}(\varepsilon^{-1})$.

6. Concluding remarks

In this paper we have derived discrete wave action conservation laws for the discrete variational/multisymplectic Euler method and the class of multisymplectic Runge-Kutta box schemes. Within the variational framework it is also possible to derive

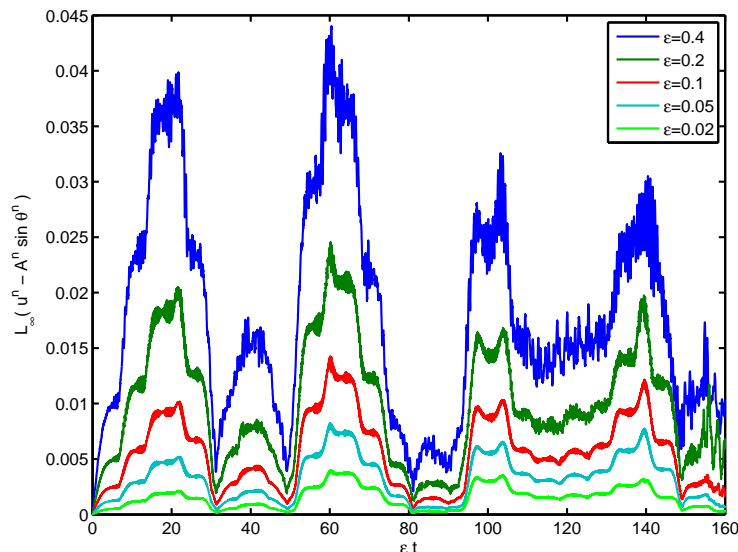


Figure 3. Approximation of the solution by the discrete modulation equations as a function of ε .

discrete modulation equations. Numerical experiments confirm that wave action is conserved to machine precision and also suggest that the discrete modulation equations approximate the numerical solution to order $\mathcal{O}(\varepsilon)$ for intervals of $\mathcal{O}(\varepsilon^{-1})$. Since the discrete modulation equations can be written in terms of slowly varying amplitude, wavenumber and frequency, it might be feasible to solve these on a coarse mesh.

Because the discrete variational framework also gives access to the full modulation equations, a general development of wave action for this class would be desirable.

The wave action conservation laws of this paper apply more generally to discretized nonlinear PDEs, and in the case of the box schemes, also to nonuniform space-time grids. To actually compute the wave action, however, one must have an explicit expression for a periodic wave train, just as in the continuous case.

Wave action is the generalization to PDEs of the concept of an adiabatic invariant. The classical example of an adiabatic invariant is the slowly modulated harmonic oscillator, obtained from (4) by setting $\alpha \equiv 0$ (Arnold 1989). Reich has shown that symplectic integrators conserve adiabatic invariants over exponentially long times (Reich 1999, Cotter & Reich 2004), see also (Cotter 2004). Estimates of the longevity of wave action conservation for PDE discretizations are currently lacking.

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