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Journal of Geometry and Physics 35 (2000) 333–366

JOURNAL OF
GEOMETRY AND
PHYSICS

A variational approach to second-order multisymplectic field theory

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Received 22 November 1999; received in revised form 26 January 2000

Abstract

This paper presents a geometric-variational approach to continuous and discrete second-order field theories following the methodology of [Marsden, Patrick, Shkoller, *Comm. Math. Phys.* 199 (1998) 351–395]. Staying entirely in the Lagrangian framework and letting Y denote the configuration fiber bundle, we show that both the multisymplectic structure on J^3Y as well as the Noether theorem arise from the first variation of the action function. We generalize the multisymplectic form formula derived for first-order field theories in [Marsden, Patrick, Shkoller, *Comm. Math. Phys.* 199 (1998) 351–395], to the case of second-order field theories, and we apply our theory to the Camassa–Holm (CH) equation in both the continuous and discrete settings. Our discretization produces a multisymplectic-momentum integrator, a generalization of the Moser–Veselov rigid body algorithm to the setting of nonlinear PDEs with second-order Lagrangians. © 2000 Elsevier Science B.V. All rights reserved.

MSC: 49S05; 70H30

Subj. Class: Classical field theory

Keywords: Multisymplectic geometry; Shallow water equations

1. Introduction

This paper continues the development of the variational approach to multisymplectic field theory introduced in [12]. In that paper, only first-order field theories were considered. Herein, we shall focus on second-order field theories, i.e., those field theories governed by Lagrangians that depend on the space–time location, the field, and its first and second partial derivatives.

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Multisymplectic geometry and its applications to covariant field theory and nonlinear partial differential equations (PDEs) has a rich and interesting history that we shall not discuss in this paper; rather, we refer the reader to [5–12] and the references therein. The covariant multisymplectic approach is the field-theoretic generalization of the symplectic approach to classical mechanics. The configuration manifold Q of classical Lagrangian mechanics is replaced by a fiber bundle $Y \rightarrow X$ over the $(n + 1)$ -dimensional space–time manifold X , whose sections are the physical fields of interest; the Lagrangian phase space is TQ in Lagrangian mechanics, whereas for k th-order field theories, the role of phase space is played by the k th jet bundle of Y , $J^k Y$, thus reflecting the additional dependence of the fields on spatial variables.

For a given smooth Lagrangian $L : TQ \rightarrow \mathbb{R}$, there is a distinguished symplectic 2-form ω_L on TQ , whose Hamiltonian vector field is the solution of the Euler–Lagrange equations of Lagrangian mechanics. Lagrangian field theories, on the other hand, governed by covariant Lagrangians $\mathcal{L} : J^k Y \rightarrow \Lambda^{n+1}(X)$, can be completely described by the multisymplectic $(n + 2)$ -form $\Omega_{\mathcal{L}}$ on $J^{2k-1} Y$, the field-theoretic analog of the symplectic 2-form ω_L of classical mechanics. In the case that X is one-dimensional, $\Omega_{\mathcal{L}}$ reduces to the usual time-dependent 2-form of classical nonautonomous mechanics (see [13]).

Traditionally, the symplectic 2-form ω_L as well as the multisymplectic $(n + 2)$ -form $\Omega_{\mathcal{L}}$ are constructed on the Lagrangian side, using the pull-back by the Legendre transform of canonical differential forms on the dual or Hamiltonian side. Recently, however, Marsden et al. [12] have shown that for first-order field theories wherein $\mathcal{L} : J^1 Y \rightarrow \Lambda^{n+1}(X)$, $\Omega_{\mathcal{L}} = d\Theta_{\mathcal{L}}$ arises as the boundary term in the first variation of the action $\int_X \mathcal{L} \circ j^1 \phi$ for smooth mappings $\phi : X \rightarrow Y$. This method is advantageous to the traditional approach in that

1. a complete geometric theory can be derived while staying entirely on the Lagrangian side, and
2. multisymplectic structure can be obtained in non-standard settings such as discrete field theory.

The purpose of this paper is to generalize the results of Marsden et al. [12] to the case that $\mathcal{L} : J^2 Y \rightarrow \Lambda^{n+1}(X)$. In Section 2, we prove in Theorem 2.1, that a unique multisymplectic $(n + 2)$ -form arises as the boundary term of the first variation of the action function. We then prove in Theorem 2.2 the multisymplectic form formula for second-order field theories, a covariant generalization of the fact that in conservative mechanics, the flow preserves the symplectic structure. We then obtain the covariant Noether theorem for second-order field theories, by taking the first variation of the action function, restricted to the space of solutions of the covariant Euler–Lagrange equations.

In Section 3, we use our abstract geometric theory on the Camassa–Holm (CH) equation, a model of shallow water waves that simultaneously exhibits solitary wave interaction and wave-breaking. We show that the multisymplectic form formula produces a new conservation law ideally suited to study wave instability, and connect our intrinsic theory with Bridges’ theory of multisymplectic structures (see [1,12]).

Section 4 is devoted to the discretization of second-order field theories. We are able to use our general theory to produce numerical algorithms for nonlinear PDEs governed by

second-order Lagrangians; these naturally respect a discrete multisymplectic form formula and a discrete Noether theorem. Again, we demonstrate this methodology on the CH equation. Of course, we would have been pleased to see that the multisymplectic numerical schemes proposed here, in practice, capture dynamics of the signature “peakon” solutions of the CH equation. However, the practical applications of these new numerical schemes are beyond the scope of the present work.

2. Variational principles for second-order classical field theory

2.1. Multisymplectic geometry

In this section, we review some aspects of the following multisymplectic geometry [9,11–13].

Let X be an orientable $(n + 1)$ -dimensional manifold (which in applications is usually space–time) and let $\pi_{XY} : Y \rightarrow X$ be a fiber bundle over X . Sections $\phi : X \rightarrow Y$ of this *covariant configuration bundle* will be the physical fields. The space of sections of π_{XY} will be denoted by $C^\infty(\pi_{XY})$ or by $C^\infty(Y)$. The vertical bundle VY is the subbundle $\ker T\pi_{XY}$ of TY , where $T\pi_{XY}$ denotes the tangent map of the π_{XY} .

If X has local coordinates x^μ , $\mu = 1, 2, \dots, n, 0$, adapted coordinates on Y are y^A , $A = 1, \dots, N$, along the fibers $Y_x := \pi_{XY}^{-1}(x)$, where $x \in X$ and N is the fiber dimension of Y .

$J^k Y$ denotes the k th jet bundle of Y , and this bundle may be defined inductively by $J^k(\dots(J^1 Y))$. Recall that the first jet bundle $J^1 Y$ is the affine bundle over Y whose fiber over $y \in Y_x$ consists of those linear mappings $\gamma : T_x X \rightarrow T_y Y$ satisfying

$$T\pi_{XY} \circ \gamma = \text{Identity on } T_x X.$$

Coordinates (x^μ, y^A) on π_{XY} induce coordinates y_μ^A on the fibers of $J^1 Y$. Given $\phi \in C^\infty(Y)$, its tangent map at $x \in X$, denoted by $T_x \phi$ is an element of $J^1 Y_{\phi(x)}$. Therefore, the map $x \rightarrow T_x \phi$ defines a section of $J^1 Y$ regarded as a bundle over X . This section is denoted by $j^1(\phi)$ and is called the first jet of ϕ , or the first prolongation of ϕ . In coordinates, $j^1(\phi)$ is given by

$$x^\mu \mapsto (x^\mu, \phi^A(x^\mu), \partial_\nu \phi^A(x^\mu)),$$

where $\partial_\nu = \partial/\partial x^\nu$. A section of the bundle $J^1 Y \rightarrow X$ which is the first prolongation of the section of $Y \rightarrow X$ is said to be holonomic.

The first jet bundle $J^1 Y$ is the appropriate configuration bundle for first-order field theories, i.e., field theories governed by Lagrangians which only depend on the space–time position, the field, and the first partial derivatives of the field. Herein, we shall focus on second-order field theories that are governed by Lagrangians which additionally depend on the second partial derivatives of the fields; thus, in second-order field theories, the Lagrangian is defined on $J^2 Y \equiv J^1(J^1 Y)$. Let us be more specific.

Definition 2.1. The second jet bundle is the affine bundle over $J^1 Y$ whose fiber at $\gamma \in J^1 Y_y$ consists of linear mappings $s : T_x X \rightarrow T_\gamma J^1 Y$ satisfying

$$T\pi_{X,J^1Y} \circ s = \text{Identity on } T_x X.$$

One can define the second jet prolongation of a section $\phi : X \rightarrow Y$, $j^2(\phi)$, as $j^1(j^1(\phi))$, that is a map $x \mapsto T_x j^1(\phi)$, where $j^1(\phi)$ is regarded as a section of J^1Y over X . This map defines a section of J^2Y regarded as a bundle over X with $j^2(\phi)(x)$ being a linear map from $T_x X$ into $T_{j^1(\phi)(x)} J^1Y$. In coordinates, $j^2(\phi)$ is given by

$$x^\mu \mapsto (x^\mu, \phi^A(x^\mu), \partial_{\mu_1} \phi^A(x^\mu), \partial_{\mu_2} \partial_{\mu_1} \phi^A(x^\mu)).$$

We shall also use the notation $\phi^A_{,\mu_1\mu_2} \equiv \partial_{\mu_2} \partial_{\mu_1} \phi^A$ for second partial derivatives. A section ρ of $J^2Y \rightarrow X$ is said to be 2-holonomic if $\rho = j^2(\pi_{Y,J^2Y} \circ \rho)$. Continuing inductively, one defines the k th jet prolongation of ϕ , $j^k(\phi)$, as $j^1(\dots(j^1(\phi)))$.

Consider a second-order Lagrangian density defined as a fiber-preserving map $\mathcal{L} : J^2Y \rightarrow \Lambda^{n+1}(X)$, where $\Lambda^{n+1}(X)$ is the bundle of $(n + 1)$ -forms on X . In coordinates, we write

$$\mathcal{L}(s) = L(x^\mu, y^A, y^A_{\mu_1}, y^A_{\mu_1\mu_2})\omega,$$

where $\omega = dx^1 \wedge \dots \wedge dx^n \wedge dx^0$.

For any k th-order Lagrangian field theory, the fundamental geometric structure is the Cartan form $\Theta_{\mathcal{L}}$; this is an $(n + 1)$ -form defined on $J^{2k-1}Y$ (see [9]). For second-order field theories, the Cartan form is defined on J^3Y , the covariant analog of the phase space in mechanics. The Euler–Lagrange equations may be written intrinsically as

$$(j^3\phi)^*(V \lrcorner d\Theta_{\mathcal{L}}) = 0 \quad \forall V \in T(J^3Y), \tag{2.1}$$

where \lrcorner denotes the interior product. Traditionally, the Cartan form is defined using the pull-back by the covariant Legendre transform of the canonical multisymplectic $(n+1)$ -form on the affine dual of $J^{2k-1}Y$ (see [9,11,13]). In local coordinates, the Cartan form on J^3Y is given by

$$\begin{aligned} \Theta_{\mathcal{L}} = & \left(\frac{\partial L}{\partial y^A_v} - D_\mu \left(\frac{\partial L}{\partial y^A_{v\mu}} \right) \right) dy^A \wedge \omega_v + \frac{\partial L}{\partial y^A_{v\mu}} dy^A_v \wedge \omega_\mu \\ & + \left(L - \frac{\partial L}{\partial y^A_v} y^A_v + D_\mu \left(\frac{\partial L}{\partial y^A_{v\mu}} \right) y^A_v - \frac{\partial L}{\partial y^A_{v\mu}} y^A_{v\mu} \right) \omega, \end{aligned} \tag{2.2}$$

where $\omega_v = \partial_v \lrcorner \omega$ and $\omega_{\mu v} = \partial_v \lrcorner \partial_\mu \lrcorner \omega$, etc. For a k th-order function $f \in C^\infty(J^kY, \mathbb{R})$, the formal partial derivative of f in the direction x^μ , denoted by $D_\mu f$, is defined by $(j^{k+1}\phi)^*(D_\mu f) = \partial_\mu(f \circ j^k\phi)$ for all $\phi \in C^\infty(Y)$, and is a smooth function on $J^{k+1}Y$. In jet charts

$$D_v f = \partial_v f + \frac{\partial f}{\partial y^A_v} y^A_v + \dots + \frac{\partial f}{\partial y^A_{\mu_1 \dots \mu_k}} y^A_{\mu_1 \dots \mu_k v}. \tag{2.3}$$

In the next section, we shall prove that the Cartan form arises as the boundary term in the Lagrangian variational principle.

2.2. Variational route to the multisymplectic form

In this section, we show that a multisymplectic structure is obtained by taking the derivative of an action functional, and use this structure to prove the multisymplectic counterpart of the fact that in conservative mechanics, the flow of a mechanical system consists of symplectic maps.

Let U be a smooth manifold with (piecewise) smooth closed boundary. Define the set of smooth maps

$$\mathcal{C}^\infty = \{\phi : U \rightarrow Y \mid \pi_{XY} \circ \phi : U \rightarrow X \text{ is an embedding}\}.$$

For each $\phi \in \mathcal{C}^\infty$ set $\phi_X := \pi_{XY} \circ \phi$ and $U_X := \phi_X(U)$ so that $\phi_X : U \rightarrow U_X$ is a diffeomorphism. Let \mathcal{C} denote the closure of \mathcal{C}^∞ in some Hilbert or Banach space norm. The choice of topology is not crucial in this paper, and one may assume that all fields are smooth. The tangent space to the manifold \mathcal{C} at a point $\phi \in \mathcal{C}$ is given by

$$\{V \in \mathcal{C}^\infty(X, TY) \mid \pi_{Y, TY} \circ V = \phi \text{ and } V_X := T\pi_{XY} \circ V \circ \phi_X^{-1} \text{ is a vector field on } X\}.$$

Consider G , the Lie group of π_{XY} -bundle automorphisms $\eta_Y : Y \rightarrow Y$ covering diffeomorphisms $\eta_X : X \rightarrow X$.

Definition 2.2. The group action $\Phi : G \times \mathcal{C} \rightarrow \mathcal{C}$ is given by

$$\Phi(\eta_Y, \phi) = \eta_Y \circ \phi.$$

Note that $(\eta_Y \circ \phi)_X = \eta_X \circ \phi_X$, and if $\phi \circ \phi_X^{-1} \in \mathcal{C}^\infty(\pi_{U_X, Y})$, then $(\eta_Y \circ \phi) \circ \phi_X^{-1} \circ \eta_X^{-1} \in \mathcal{C}^\infty(\pi_{\eta_X(U_X), Y})$.

The fundamental problem of the classical calculus of variations is to extremize the action functional over the space of sections of $Y \rightarrow X$.

Definition 2.3. The action functional $\mathcal{S} : \mathcal{C} \rightarrow \mathbb{R}$ is given by

$$\mathcal{S}(\phi) = \int_{U_X} \mathcal{L}(j^2(\phi \circ \phi_X^{-1})) \quad \forall \phi \in \mathcal{C}. \quad (2.4)$$

Definition 2.4. $\phi \in \mathcal{C}$ is said to be an extremum of \mathcal{S} if

$$\left. \frac{d}{d\lambda} \right|_{\lambda=0} \mathcal{S}(\Phi(\eta_Y^\lambda, \phi)) = 0$$

for all smooth paths $\lambda \mapsto \eta_Y^\lambda$ in G , where for each λ , η_Y^λ covers η_X^λ .

One may associate to each $\phi^\lambda \in \mathcal{C}$, the section of Y given by $\eta_Y^\lambda \circ (\phi \circ \phi_X^{-1}) \circ (\eta_X^\lambda)^{-1}$, namely $\eta_Y^\lambda \circ (\phi \circ \phi_X^{-1}) \circ (\eta_X^\lambda)^{-1}$ maps $U_X^\lambda := \eta_X^\lambda \circ \phi_X(U)$ into $\phi^\lambda(U)$.

If we choose the curve ϕ^λ such that $\phi^0 = \phi$ and $(d/d\lambda)|_{\lambda=0} \Phi(\eta_Y^\lambda, \phi) = V$, then we have that $V = (d/d\lambda)|_{\lambda=0} \phi^\lambda$ and $V_X = (d/d\lambda)|_{\lambda=0} \eta_X^\lambda$. This will be used in the following equation:

$$\begin{aligned}
d\mathcal{S}_\phi \cdot V &= \frac{d}{d\lambda} \Big|_{\lambda=0} \mathcal{S}(\phi^\lambda) = \frac{d}{d\lambda} \Big|_{\lambda=0} \int_{U_X^\lambda} \mathcal{L}(j^2(\phi^\lambda \circ (\phi_X^\lambda)^{-1})) \\
&= \int_{U_X} \frac{d}{d\lambda} \Big|_{\lambda=0} \mathcal{L}(j^2(\phi^\lambda \circ (\phi_X^\lambda)^{-1})) + \int_{U_X} \frac{d}{d\lambda} \Big|_{\lambda=0} (\eta_X^\lambda)^* \mathcal{L}(j^2(\phi \circ \phi_X^{-1})) \\
&= \int_{U_X} \frac{d}{d\lambda} \Big|_{\lambda=0} \mathcal{L}(j^2(\phi^\lambda \circ (\phi_X^\lambda)^{-1})) + \int_{U_X} \mathfrak{L}_{V_X} \mathcal{L}(j^2(\phi \circ \phi_X^{-1})), \quad (2.5)
\end{aligned}$$

where $*$ stands for the pull-back, and \mathfrak{L} denotes the Lie derivative.

Now, let $VY \subset TY$ be the vertical subbundle; this is the bundle over Y whose fibers are given by

$$V_y Y = \{v \in T_y Y \mid T\pi_{XY} \cdot v = 0\}.$$

For each $\gamma \in J^1 Y_y$ there exists a natural splitting $T_y Y = \text{image } \gamma \oplus V_y Y$. For example, for a vector $V \in T_\phi \mathcal{C}$, let $\gamma = j^1(\phi \circ \phi_X^{-1})$, $V^h := \gamma(V_X)$, and $V^v := V \circ \phi_X^{-1} - V^h$. Then

$$T\pi_{XY} \circ V^h = T\pi_{XY} \circ \gamma(V_X) = \text{id}_{TX}(V_X) = V_X.$$

On the other hand, by definition, $V_X = T\pi_{XY} \circ V \circ \phi_X^{-1}$. Therefore, $T\pi_{XY} \cdot V^v = 0$ which confirms that any vector $V \in T_\phi \mathcal{C}$ may be decomposed into its horizontal component

$$V^h = T(\phi \circ \phi_X^{-1}) \cdot V_X, \quad (2.6)$$

and its vertical component

$$V^v = V \circ \phi_X^{-1} - V^h. \quad (2.7)$$

Remark 2.1. Notice that $V(x) \in T_{\phi(x)} Y$ for all $x \in U$, while V^h and V^v are vector fields on $U_X = \phi_X(U)$.

Next, we define prolongations of automorphisms η_Y of Y and of elements $V \in T_\phi \mathcal{C}$.

Definition 2.5. Given an automorphism η_Y of $Y \rightarrow X$, its first prolongation $j^1(\eta_Y) : J^1 Y \rightarrow J^1 Y$ is defined via

$$j^1(\eta_Y)(\gamma) = T\eta_Y \circ \gamma \circ T\eta_X^{-1}.$$

If $\gamma : T_x X \rightarrow T_y Y$, then $j^1(\eta_Y)(\gamma) : T_{\eta_X(x)} X \rightarrow T_{\eta_Y(y)} Y$, with local coordinate expression

$$j^1(\eta_Y)(\gamma) = \left(\eta_X^\mu, \eta_Y^A, \left(\frac{\partial \eta_Y^A}{\partial x^\nu} + \gamma_\nu^B \frac{\partial \eta_Y^A}{\partial y^B} \right) \frac{(\eta_X^{-1})^\nu}{\partial x^\mu} \right). \quad (2.8)$$

To define the first prolongation of a vector $V \in T_\phi \mathcal{C}$, denoted by $j^1(V)$, let η_Y^λ be a flow of a vector field v on Y with $v \circ \phi = V$.

Definition 2.6. The first prolongation $j^1(V)$ of V is a vector field on $J^1 Y$ given by

$$j^1(V) = \frac{d}{d\lambda} \Big|_{\lambda=0} j^1(\eta_Y^\lambda).$$

If in a coordinate chart $V = (V^\mu, V^A)$; identifying V with $V \circ \phi_X^{-1}$, we see that (2.8) yields the following local expression for $j^1(V)(\gamma)$:

$$j^1(V)(\gamma) = \left(V^\mu, V^A, \frac{\partial V^A}{\partial x^\mu} + \frac{\partial V^A}{\partial y^B} \gamma_\mu^B - \gamma_\nu^A \frac{\partial V^\nu}{\partial x^\mu} \right). \tag{2.9}$$

Using induction, one can define the k th prolongation of an automorphism η_Y and the k th prolongation of a vector $V \in T_\phi \mathcal{C}$ for all $k \geq 1$, and these will be denoted by $j^k(\eta_Y)$ and $j^k(V)$, respectively.

Definition 2.7. For a k th-order function $f \in C^\infty(J^k Y, \mathbb{R})$, the variational derivative of f is the function on $J^{2k} Y$ given by

$$\frac{\delta f}{\delta y^A} = \sum_{s=0}^k (-1)^s D_{\mu_1} \cdots D_{\mu_s} \left(\frac{\partial f}{\partial y_{\mu_1 \cdots \mu_s}^A} \right).$$

In particular, for a second-order function $f \in C^\infty(J^2 Y, \mathbb{R})$, the variational derivative of f is the function on $J^4 Y$ given by

$$\frac{\delta f}{\delta y^A} = \frac{\partial f}{\partial y^A} - D_\nu \left(\frac{\partial f}{\partial y_\nu^A} \right) + D_\nu D_\mu \left(\frac{\partial f}{\partial y_{\nu\mu}^A} \right).$$

Throughout the paper we will use both $V \lrcorner \alpha$ and $\mathbf{i}_V \alpha$ for the interior product.

Definition 2.8. Let $\mathcal{C}^4 = \{j^4(\phi \circ \phi_X^{-1}) | \phi \in \mathcal{C}\}$.

Theorem 2.1. Given a smooth Lagrangian density $\mathcal{L} : J^2 Y \rightarrow \Lambda^{n+1}(X)$, there exist a unique $\Psi \in \Lambda^{n+2}(J^4 Y)$ given by

$$\Psi = \frac{\delta L}{\delta y^A} dy^A \wedge \omega,$$

a unique map $\mathcal{D}_{\text{EL}} \mathcal{L} \in C^\infty(\mathcal{C}^4, T^* \mathcal{C} \otimes \Lambda^{n+1}(X))$ given by

$$\mathcal{D}_{\text{EL}} \mathcal{L}(\phi) \cdot V = j^4(\phi \circ \phi_X^{-1})^* \left(\frac{\delta L}{\delta y^A} \mathbf{i}_V(dy^A \wedge \omega) \right), \tag{2.10}$$

and a unique differential form $\Theta_{\mathcal{L}} \in \Lambda^{n+1}(J^3 Y)$ given by

$$\begin{aligned} \Theta_{\mathcal{L}} = & \left(\frac{\partial L}{\partial y_\nu^A} - D_\mu \left(\frac{\partial L}{\partial y_{\nu\mu}^A} \right) \right) dy^A \wedge \omega_\nu + \frac{\partial L}{\partial y_{\nu\mu}^A} dy_\nu^A \wedge \omega_\mu \\ & + \left(L - \frac{\partial L}{\partial y_\nu^A} y_\nu^A + D_\mu \left(\frac{\partial L}{\partial y_{\nu\mu}^A} \right) y_\nu^A - \frac{\partial L}{\partial y_{\nu\mu}^A} y_{\nu\mu}^A \right) \omega \end{aligned} \tag{2.11}$$

such that $j^3(\phi \circ \phi_X^{-1})^* \Theta_{\mathcal{L}} = \mathcal{L} \circ j^2(\phi \circ \phi_X^{-1})$ for any $\phi \in \mathcal{C}$, and the variation of the action functional \mathcal{S} is expressed by the following formula: for any $V \in T_\phi \mathcal{C}$ and any open subset U_X of X such that $\overline{U_X} \cap \partial X = \emptyset$,

$$d\mathcal{S}_\phi \cdot V = \int_{U_X} \mathcal{D}_{\text{EL}} \mathcal{L}(\phi) \cdot V + \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \Theta_{\mathcal{L}}]. \tag{2.12}$$

Furthermore,

$$\mathcal{D}_{\text{EL}}\mathcal{L}(\phi) \cdot V = j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \Omega_{\mathcal{L}}] \text{ in } U_X, \quad (2.13)$$

where $\Omega_{\mathcal{L}} = d\Theta_{\mathcal{L}}$ is the multisymplectic form on J^3Y . The variational principle (2.12) yields the Euler–Lagrange equations (2.1) on the interior of the domain, which in coordinates are given by

$$\begin{aligned} \frac{\partial L}{\partial y^A} (j^2(\phi \circ \phi_X^{-1})) - \frac{\partial}{\partial x^\nu} \left(\frac{\partial L}{\partial y_\nu^A} (j^2(\phi \circ \phi_X^{-1})) \right) \\ + \frac{\partial^2}{\partial x^\nu \partial x^\mu} \left(\frac{\partial L}{\partial y_{\nu\mu}^A} (j^2(\phi \circ \phi_X^{-1})) \right) = 0, \end{aligned} \quad (2.14)$$

while the form $\Theta_{\mathcal{L}}$ naturally arises in the boundary term and matches the definition of the Cartan form given in (2.2).

Proof. The proof proceeds in three steps. We begin by computing the first variation using (2.5). Then we show that the boundary term yields the Cartan form. Lastly, we verify the statements related to the interior integral.

Choose $U_X = \phi_X(U)$ small enough so that it is contained in a coordinate chart. If in these coordinates $V = (V^\mu, V^A)$, then along $\phi \circ \phi_X^{-1}$, the coordinate expressions for V_X , V^h , V^v are written as

$$\begin{aligned} V_X &= V^\mu \frac{\partial}{\partial x^\mu}, & V^h &= V^\mu \frac{\partial}{\partial x^\mu} + V^\mu \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\mu} \frac{\partial}{\partial y^A}, \\ V^v &= (V^v)^A \frac{\partial}{\partial y^A} := \left(V^A - V^\mu \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\mu} \right) \frac{\partial}{\partial y^A}. \end{aligned} \quad (2.15)$$

Using the Cartan formula we first compute the second term on the right-hand side of (2.5)

$$\begin{aligned} \int_{U_X} \mathfrak{L}_{V_X} \mathcal{L}(j^2(\phi \circ \phi_X^{-1})) &= \int_{U_X} \mathfrak{L}_{V_X} (L\omega) = \int_{U_X} \mathbf{d}\mathbf{i}_{V_X} (L\omega) + \mathbf{i}_{V_X} d(L\omega) \\ &= \int_{\partial U_X} L \mathbf{i}_{V_X} \omega = \int_{\partial U_X} L V^\theta \omega_\theta. \end{aligned} \quad (2.16)$$

Using (2.7), and the local expression for the vertical vector field V^v , we have that

$$\begin{aligned} \int_{U_X} \frac{d}{d\lambda} \Big|_{\lambda=0} \mathcal{L}(j^2(\phi^\lambda \circ (\phi_X^\lambda)^{-1})) \\ = \int_{U_X} \left[\frac{\partial L}{\partial y^A} (j^2(\phi \circ \phi_X^{-1})) (V^v)^A + \frac{\partial L}{\partial y_\nu^A} (j^2(\phi \circ \phi_X^{-1})) (V^v)_{,\nu}^A \right. \\ \left. + \frac{\partial L}{\partial y_{\nu\mu}^A} (j^2(\phi \circ \phi_X^{-1})) (V^v)_{,\nu\mu}^A \right] \omega. \end{aligned} \quad (2.17)$$

In the following, we shall use $D_\nu f$ for the formal partial derivative of a function f (see (2.3)), and $(\partial f / \partial x^\nu)$ will denote $(\partial / \partial x^\nu)(f \circ j^2(\phi \circ \phi_X^{-1}))$. Integrating (2.17) by parts, we obtain that

$$\int_{U_X} \left[\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right] (V^v)^A \omega$$

$$+ \int_{U_X} \left(\frac{\partial L}{\partial y_v^A} (V^v)^A \right)_{,v} \omega + \int_{U_X} \left(\frac{\partial L}{\partial y_{v\mu}^A} (V^v)^A \right)_{,\mu} \omega$$

$$- \int_{U_X} \left(\frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) (V^v)^A \right)_{,v} \omega.$$

Using the fact $f_{,v}\omega = d(f\omega_v)$, applying the Stoke’s formula $\int_U d\alpha = \int_{\partial U} \alpha$, and combining the last calculation with (2.16), we obtain

$$dS_\phi \cdot V = \int_{U_X} \left[\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right] (V^v)^A \omega$$

$$+ \int_{\partial U_X} \left(\frac{\partial L}{\partial y_v^A} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) (V^v)^A \omega_v + \frac{\partial L}{\partial y_{v\mu}^A} (V^v)^A_{,v} \omega_\mu + L V^\theta \omega_\theta.$$

(2.18)

□

Definition 2.9. A form α on $J^k Y$ is contact, if $(j^k \phi)^* \alpha = 0$ for all $\phi \in C^\infty(Y)$.

Lemma 2.1. For a smooth Lagrangian density $\mathcal{L} : J^2 Y \rightarrow \Lambda^{n+1}(X)$ there exists a unique differential form $\Theta_{\mathcal{L}} \in \Lambda^{n+1}(J^3 Y)$ defined by (2.11) such that the boundary integral in (2.18) is equal to

$$\int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \Theta_{\mathcal{L}}].$$

Furthermore, $\Theta_{\mathcal{L}}$ can be written as a sum of $L\omega$ and a linear combination of a system of contact forms on $J^2 Y$ with coefficients being functions on $J^3 Y$.

Proof of Lemma 2.1. Let $W = (W^\mu, W^A, W_\mu^A, W_{\mu\nu}^A, W_{\mu\nu\theta}^A)$ be an arbitrary vector field on $J^3 Y$, and let $\varphi := j^3(\phi \circ \phi_X^{-1})$, a map from U_X to $J^3 Y$. Then one computes

$$\mathbf{i}_W(dy^A \wedge \omega_v) = W^A \omega_v - W^\theta dy^A \wedge \omega_{v\theta},$$

$$\mathbf{i}_W(dy_v^A \wedge \omega_\mu) = W_v^A \omega_\mu - W^\theta dy_v^A \wedge \omega_{\mu\theta},$$

$$\varphi^* \mathbf{i}_W(dy^A \wedge \omega_v) = W^A \omega_v - W^\theta \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\mu} dx^\mu \wedge \omega_{v\theta}.$$

Using the formula

$$dx^\mu \wedge \omega_{v\theta} = \begin{cases} 0 & \text{if } \mu \neq v, \theta, \\ \omega_v & \text{if } \mu = \theta, \\ -\omega_\theta & \text{if } \mu = v, \end{cases} \tag{2.19}$$

one finds that

$$\varphi^* \mathbf{i}_W (dy^A \wedge \omega_v) = W^A \omega_v - W^\theta \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\theta} \omega_v + \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^v} W^\theta \omega_\theta.$$

Similarly,

$$\varphi^* \mathbf{i}_W (dy_v^A \wedge \omega_\mu) = W_v^A \omega_\mu - W^\theta \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\theta \partial x^v} \omega_\mu + \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\mu \partial x^v} W^\theta \omega_\theta.$$

Thus, if we let $W = j^3(V)$, use (2.9), and recall the local expression (2.15) for $(V^v)^A$, we obtain that

$$\begin{aligned} \varphi^* \mathbf{i}_{j^3(V)} (dy^A \wedge \omega_v) &= (V^v)^A \omega_v + \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^v} V^\theta \omega_\theta, \\ \varphi^* \mathbf{i}_{j^3(V)} (dy_v^A \wedge \omega_\mu) &= (V^v)^A_{,v} \omega_\mu + \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\mu \partial x^v} V^\theta \omega_\theta. \end{aligned}$$

Next, observe that $V^\theta \omega_\theta = \mathbf{i}_V \omega$. Also,

$$\frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^v} = j^3(\phi \circ \phi_X^{-1})^* y_v^A, \quad \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\mu \partial x^v} = j^3(\phi \circ \phi_X^{-1})^* y_{v\mu}^A.$$

These observations together with the previous identities imply the following important formulas:

$$\begin{aligned} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner (dy_v^A \wedge \omega_\mu - y_{v\mu}^A \omega)] &= (V^v)^A_{,v} \omega_\mu, \\ j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner (dy^A \wedge \omega_v - y_v^A \omega)] &= (V^v)^A \omega_v. \end{aligned} \quad (2.20)$$

Substituting these formulas into the boundary integral of the variational principle (2.18), we obtain that

$$\begin{aligned} &\int_{\partial U_X} \left(\frac{\partial L}{\partial y_v^A} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) (V^v)^A \omega_v + \frac{\partial L}{\partial y_{v\mu}^A} (V^v)^A_{,v} \omega_\mu + L V^\theta \omega_\theta \\ &= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* \left\{ j^3(V) \lrcorner \left[\left(\frac{\partial L}{\partial y_v^A} - D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) (dy^A \wedge \omega_v - y_v^A \omega) \right. \right. \\ &\quad \left. \left. + \frac{\partial L}{\partial y_{v\mu}^A} (dy_v^A \wedge \omega_\mu - y_{v\mu}^A \omega) + L \omega \right] \right\} \\ &= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* \left\{ j^3(V) \lrcorner \left[\left(\frac{\partial L}{\partial y_v^A} - D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) dy^A \wedge \omega_v \right. \right. \\ &\quad \left. \left. + \frac{\partial L}{\partial y_{v\mu}^A} dy_v^A \wedge \omega_\mu + \left(L - \frac{\partial L}{\partial y_v^A} y_v^A + D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) y_v^A - \frac{\partial L}{\partial y_{v\mu}^A} y_{v\mu}^A \right) \omega \right] \right\} \\ &= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \Theta_{\mathcal{L}}]. \end{aligned}$$

This proves the existence of a unique differential form $\Theta_{\mathcal{L}}$ and demonstrates how this form naturally arises in the boundary integral of the variational principle. Integration by parts

yields the boundary integral with terms that involve partial derivatives of $(V^v)^A$ of all orders up to $k - 1$ (in our case $k = 2$). Eq. (2.20) shows that each partial derivative of $(V^v)^A$ has an associated $(n + 1)$ -form on J^2Y , and substitution of these forms yields a unique differential $(n + 1)$ -form as desired. Since L and its partial derivatives are functions on J^2Y , then by (2.3), $D_\mu(\partial L/\partial y_{v\mu}^A)$ is a function on J^3Y , and therefore $\Theta_{\mathcal{L}}$ is a $(n + 1)$ -form on J^3Y .

It is easy to show that

$$j^k(\phi \circ \phi_X^{-1})^*(dy^A \wedge \omega_v - y_v^A \omega) = 0, \quad j^k(\phi \circ \phi_X^{-1})^*(dy_v^A \wedge \omega_\mu - y_{v\mu}^A \omega) = 0$$

for all integers $k \geq 2$ and for all $\phi \in \mathcal{C}$. Therefore, $dy^A \wedge \omega_v - y_v^A \omega$ and $dy_v^A \wedge \omega_\mu - y_{v\mu}^A \omega$ are contact forms on J^2Y . Hence the last statement of the lemma follows. \square

A simple computation then verifies that $\Theta_{\mathcal{L}}$ is the Cartan form so that

$$j^3(\phi \circ \phi_X^{-1})^*\Theta_{\mathcal{L}} = \mathcal{L} \circ j^2(\phi \circ \phi_X^{-1}).$$

Next, consider the interior integral of the variational principle (2.18). Since $j^k(\phi \circ \phi_X^{-1})^*\mathbf{i}_{j^k(V)}(dy^A \wedge \omega) = (V^v)^A \omega$ for all integers $k \geq 1$, we obtain that

$$\begin{aligned} & \int_{U_X} \left[\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right] (V^v)^A \omega \\ &= \int_{U_X} j^4(\phi \circ \phi_X^{-1})^*\mathbf{i}_{j^4(V)} \left[\frac{\partial L}{\partial y^A} - D_v \left(\frac{\partial L}{\partial y_v^A} \right) + D_v D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right] dy^A \wedge \omega \\ &= \int_{U_X} j^4(\phi \circ \phi_X^{-1})^*\mathbf{i}_{j^4(V)} \left(\frac{\delta L}{\delta y^A} dy^A \wedge \omega \right), \end{aligned} \tag{2.21}$$

where $\delta L/\delta y^A$ is the variational derivative of L in the direction y^A (see Definition 2.7). Since L is a function of second-order by hypothesis, then its variational derivative is a function on J^4Y . Therefore, the form $\Psi \equiv (\delta L/\delta y^A) dy^A \wedge \omega$ is an $(n + 2)$ -form on J^4Y . Moreover, the integrand in (2.21) written as $j^4(\phi \circ \phi_X^{-1})^*((\delta L/\delta y^A)\mathbf{i}_V(dy^A \wedge \omega))$ defines a unique smooth section $\mathcal{D}_{EL}\mathcal{L} \in C^\infty(\mathcal{C}^4, T^*\mathcal{C} \otimes \Lambda^{n+1}(X))$ as desired in the statement of the theorem. Now we shall prove the following lemma.

Lemma 2.2. *The forms $\Omega_{\mathcal{L}} = d\Theta_{\mathcal{L}}$ and $\Psi = (\delta L/\delta y^A) dy^A \wedge \omega$ satisfy the following relationship:*

$$j^4(\phi \circ \phi_X^{-1})^*\mathbf{i}_{j^4(V)}\Psi = j^3(\phi \circ \phi_X^{-1})^*\mathbf{i}_{j^3(V)}\Omega_{\mathcal{L}} \tag{2.22}$$

for all $\phi \in \mathcal{C}$ and all vectors $V \in TC$.

Furthermore, a necessary condition for $\phi \in \mathcal{C}$ to be an extremum of the action functional S is that

$$j^3(\phi \circ \phi_X^{-1})^*\mathbf{i}_W\Omega_{\mathcal{L}} = 0 \tag{2.23}$$

for all vector fields W on J^3Y , which is equivalent to

$$j^4(\phi \circ \phi_X^{-1})^*\mathbf{i}_V\Psi = 0 \tag{2.24}$$

for all vector fields V on J^4Y .

Proof of Lemma 2.2. The proof will involve some lengthy computations that we partially present below. To compute $\Omega_{\mathcal{L}}$, let us write $\Theta_{\mathcal{L}}$ as

$$\Theta_{\mathcal{L}} = \left(\frac{\partial L}{\partial y_v^A} - D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) (dy^A \wedge \omega_v - y_v^A \omega) + \frac{\partial L}{\partial y_{v\mu}^A} (dy_v^A \wedge \omega_\mu - y_{v\mu}^A \omega) + L\omega.$$

Then, for $W \in TJ^3Y$, we obtain

$$\begin{aligned} \mathbf{i}_W \Omega_{\mathcal{L}} &= W \left[\frac{\partial L}{\partial y_v^A} - D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right] (dy^A \wedge \omega_v - y_v^A \omega) \\ &\quad - d \left(\frac{\partial L}{\partial y_v^A} - D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \wedge (W^A \omega_v - W^\theta dy^A \wedge \omega_{v\theta} - y_v^A W^\theta \omega_\theta) \\ &\quad + W \left[\frac{\partial L}{\partial y_{v\mu}^A} \right] (dy_v^A \wedge \omega_\mu - y_{v\mu}^A \omega) \\ &\quad - d \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \wedge (W_v^A \omega_\mu - W^\theta dy_v^A \wedge \omega_{\mu\theta} - y_{v\mu}^A W^\theta \omega_\theta) \\ &\quad + D_\mu \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) (W_v^A \omega - W^\theta dy_v^A \wedge \omega_\theta) + \frac{\partial L}{\partial y^A} (W^A \omega - W^\theta dy^A \wedge \omega_\theta). \end{aligned}$$

The last step is to pull-back $\mathbf{i}_W \Omega_{\mathcal{L}}$ by $\varphi = j^3(\phi \circ \phi_X^{-1})$; this eliminates the terms with the contact forms. In addition, using the fact that the pull-back commutes with the exterior derivative, and applying formulas such as (2.19), we obtain that

$$\begin{aligned} \varphi^* \mathbf{i}_W \Omega_{\mathcal{L}} &= W^A \left\{ \frac{\partial L}{\partial y^A} \omega - d \left(\frac{\partial L}{\partial y_v^A} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \wedge \omega_v \right\} \\ &\quad + W^\theta \left\{ d \left(\frac{\partial L}{\partial y_v^A} - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \right. \\ &\quad \wedge \left(\frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\theta} \omega_v - \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^v} \omega_\theta + \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^v} \omega_\theta \right) \\ &\quad + d \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \wedge \left(\frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\theta \partial x^v} \omega_\mu - \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\mu \partial x^v} \omega_\theta \right. \\ &\quad \left. \left. + \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\mu \partial x^v} \omega_\theta \right) - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \frac{\partial^2(\phi \circ \phi_X^{-1})^A}{\partial x^\theta \partial x^v} \omega \right. \\ &\quad \left. - \frac{\partial L}{\partial y^A} \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\theta} \omega \right\} + W_v^A \left\{ \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \omega - d \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \wedge \omega_\mu \right\}. \end{aligned}$$

Some cancellation and further rearrangement yields

$$\begin{aligned} \varphi^* \mathbf{i}_W \Omega_{\mathcal{L}} &= W^A \left(\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \omega \\ &\quad - W^\theta \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\theta} \left(\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \omega. \end{aligned}$$

Letting $W = j^3(V)$, we have that

$$\varphi^* \mathbf{i}_{j^3(V)} \Omega_{\mathcal{L}} = (V^v)^A \left(\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \omega,$$

where the right-hand side equals $j^4(\phi \circ \phi_X^{-1})^* \mathbf{i}_{j^4(V)} \Psi$ by (2.21). Hence, the relation (2.22) is proved.

A necessary condition for $\phi \in \mathcal{C}$ to be an extremum of the action functional \mathcal{S} is that the interior integral in (2.18) vanish for all vectors $V \in T\mathcal{C}$. From the calculation above, one may readily see that it is equivalent to the condition (2.23).

Now if we let V be a vector field on J^4Y , then

$$\begin{aligned} \mathbf{i}_V \Psi &= \mathbf{i}_V \left(\frac{\delta L}{\delta y^A} dy^A \wedge \omega \right) = \frac{\delta L}{\delta y^A} \mathbf{i}_V (dy^A \wedge \omega) \\ &= \frac{\delta L}{\delta y^A} (\mathbf{i}_V (dy^A) \wedge \omega - dy^A \wedge \mathbf{i}_V \omega) = \frac{\delta L}{\delta y^A} (V^A \omega - V^\theta dy^A \wedge \omega_\theta). \end{aligned}$$

Hence,

$$\begin{aligned} j^4(\phi \circ \phi_X^{-1})^* \mathbf{i}_V \Psi &= \left(\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} \right) + \frac{\partial^2}{\partial x_v \partial x_\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} \right) \right) \\ &\quad \times \left(V^A - V^\theta \frac{\partial(\phi \circ \phi_X^{-1})^A}{\partial x^\theta} \right) \omega. \end{aligned}$$

Thus, the condition

$$j^4(\phi \circ \phi_X^{-1})^* \mathbf{i}_V \Psi = 0$$

for all vector fields V on J^4Y is equivalent to the condition (2.23). This completes the proof of the lemma. \square

Lemma 2.2 contains two equivalent conditions for $\phi \in \mathcal{C}$ to be extremal. Both conditions yield the same coordinate expression of the Euler–Lagrange equations given by

$$\begin{aligned} \frac{\partial L}{\partial y^A} (j^2(\phi \circ \phi_X^{-1})) - \frac{\partial}{\partial x^v} \left(\frac{\partial L}{\partial y_v^A} (j^2(\phi \circ \phi_X^{-1})) \right) \\ + \frac{\partial^2}{\partial x^v \partial x^\mu} \left(\frac{\partial L}{\partial y_{v\mu}^A} (j^2(\phi \circ \phi_X^{-1})) \right) = 0, \end{aligned}$$

which is the final statement of the theorem.

Remark 2.2. As one may see the proof we have presented can be generalized to Lagrangian densities on $J^k Y$. One has to modify the labeling of variables to reflect the general case. For example,

$$(V^v)_{,\mu_1 \dots \mu_l}^A \omega_\theta = \varphi^* [j^3(V) \lrcorner (dy_{\mu_1 \dots \mu_l}^A \wedge \omega_\theta - y_{\mu_1 \dots \mu_l \theta}^A \omega)],$$

where $0 \leq l \leq (k - 1)$. Then the Cartan form shall arise in the boundary integral as a linear combination of the forms above.

We shall call critical points ϕ of \mathcal{S} solutions of the Euler–Lagrange equations.

Definition 2.10. We let

$$\mathcal{P} = \{\phi \in \mathcal{C} \mid j^3(\phi \circ \phi_X^{-1})^* \mathbf{i}_W \Omega_{\mathcal{L}} = 0 \text{ for all vector fields } W \text{ on } J^3 Y\} \tag{2.25}$$

denote the space of solutions of the Euler–Lagrange equations.

We are now ready to prove the multisymplectic form formula, a covariant generalization of the symplectic flow theorem to second-order field theories.¹

2.3. Multisymplectic form formula

If ϕ^λ is a smooth curve of solutions of the Euler–Lagrange equations in \mathcal{P} (when such solutions exist), then differentiating with respect to λ at $\lambda = 0$ will give a tangent vector V to the curve at $\phi = \phi^0$. By differentiating $(d/d\lambda)|_{\lambda=0} j^3(\phi^\lambda \circ (\phi_X^\lambda)^{-1})^* [W \lrcorner \Omega_{\mathcal{L}}] = 0$, we obtain

$$j^3(\phi \circ \phi_X^{-1})^* \mathfrak{L}_{j^3(V)} [W \lrcorner \Omega_{\mathcal{L}}] = 0$$

for all vector fields W on $J^3 Y$. Therefore, if \mathcal{P} is a submanifold of \mathcal{C} , then for any $\phi \in \mathcal{P}$ we may identify $T_\phi \mathcal{P}$ with the set of vectors V that satisfy the above condition. However, we do not require \mathcal{P} to be a submanifold.

Definition 2.11. For any $\phi \in \mathcal{P}$,

$$\mathcal{F} = \{V \in T_\phi \mathcal{C} \mid j^3(\phi \circ \phi_X^{-1})^* \mathfrak{L}_{j^3(V)} [W \lrcorner \Omega_{\mathcal{L}}] = 0 \text{ for all vector fields } V \text{ on } J^3 Y\} \tag{2.26}$$

defines a set of solutions of the first variation equations of the Euler–Lagrange equations.

Theorem 2.2 (Multisymplectic form formula). *If $\phi \in \mathcal{P}$, then for all V and W in \mathcal{F} ,*

$$\int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner j^3(W) \lrcorner \Omega_{\mathcal{L}}] = 0. \tag{2.27}$$

Proof. We follow Theorem 4.1 in [12]. Define the 1-forms α_1 and α_2 on \mathcal{C} by

$$\alpha_1(\phi) \cdot V := \int_{U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \Omega_{\mathcal{L}}],$$

¹ For first-order field theories, this is Theorem 4.1 in [12].

and

$$\alpha_2(\phi) \cdot V := \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \Theta_{\mathcal{L}}],$$

so that by (2.12) and (2.13),

$$d\mathcal{S}_\phi \cdot V = \alpha_1(\phi) \cdot V + \alpha_2(\phi) \cdot V \quad \forall V \in T_\phi \mathcal{C}. \tag{2.28}$$

Furthermore,

$$d^2\mathcal{S}(\phi)(V, W) = d\alpha_1(\phi)(V, W) + d\alpha_2(\phi)(V, W) \quad \forall V, W \in T_\phi \mathcal{C}.$$

Since $d^2\mathcal{S} = 0$, we have that

$$d\alpha_1(\phi)(V, W) + d\alpha_2(\phi)(V, W) = 0 \quad \forall V, W \in T_\phi \mathcal{C}. \tag{2.29}$$

Given vectors $V, W \in T_\phi \mathcal{C}$ we may extend them to vector fields \mathcal{V}, \mathcal{W} on \mathcal{C} by fixing vector fields v, w on Y such that $V = v \circ \phi$ and $W = w \circ \phi$, and letting $\mathcal{V}(\rho) = v \circ \rho$ and $\mathcal{W}(\rho) = w \circ \rho$. If η_Y^λ covering η_X^λ is the flow of v , then $\Phi(\eta_Y^\lambda, \rho)$ is the flow of \mathcal{V} . Notice that $\mathcal{V}(\phi) = V$ and $\mathcal{W}(\phi) = W$, hence Eq. (2.29) becomes

$$d\alpha_1(\mathcal{V}, \mathcal{W})(\phi) + d\alpha_2(\mathcal{V}, \mathcal{W})(\phi) = 0.$$

Recall that for any 1-form α on \mathcal{C} and vector fields \mathcal{V}, \mathcal{W} on \mathcal{C} ,

$$d\alpha(\mathcal{V}, \mathcal{W}) = \mathcal{V}[\alpha(\mathcal{W})] - \mathcal{W}[\alpha(\mathcal{V})] - \alpha([\mathcal{V}, \mathcal{W}]). \tag{2.30}$$

Also recall that for a vector field \mathcal{V} on \mathcal{C} and a function f on \mathcal{C} , $\mathcal{V}[f] = df \cdot \mathcal{V}$. We now use the latter and (2.30) on α_2 . We have that

$$\begin{aligned} d\alpha_2(\mathcal{V}, \mathcal{W})(\phi) &= \mathcal{V}[\alpha_2(\mathcal{W})](\phi) - \mathcal{W}[\alpha_2(\mathcal{V})](\phi) - \alpha_2([\mathcal{V}, \mathcal{W}])(\phi) \\ &= [d(\alpha_2(\mathcal{W})) \cdot \mathcal{V}](\phi) - [d(\alpha_2(\mathcal{V})) \cdot \mathcal{W}](\phi) - \alpha_2(\phi) \cdot [V, W] \\ &= d(\alpha_2(\mathcal{W}))(\phi) \cdot V - d(\alpha_2(\mathcal{V}))(\phi) \cdot W - \alpha_2(\phi) \cdot [V, W]. \end{aligned} \tag{2.31}$$

Similarly,

$$d\alpha_1(\phi)(V, W) = d(\alpha_1(\mathcal{W}))(\phi) \cdot V - d(\alpha_1(\mathcal{V}))(\phi) \cdot W - \alpha_1(\phi) \cdot [V, W]. \tag{2.32}$$

Let $\phi \in \mathcal{P}$ and $\phi^\lambda = \eta_Y^\lambda \circ \phi$ be a curve in \mathcal{C} through ϕ such that

$$V = \left. \frac{d}{d\lambda} \right|_{\lambda=0} \phi^\lambda, \quad V \in \mathcal{F}.$$

Now we restrict V, W to \mathcal{F} . We shall give a detailed computation of the first term on the right-hand side of (2.31). We have that

$$\begin{aligned}
d(\alpha_2(\mathcal{W}))(\phi) \cdot V &= \left. \frac{d}{d\lambda} \right|_{\lambda=0} (\alpha_2(\mathcal{W}))(\phi^\lambda) = \left. \frac{d}{d\lambda} \right|_{\lambda=0} \alpha_2(\phi^\lambda) \cdot (w \circ \phi^\lambda) \\
&= \left. \frac{d}{d\lambda} \right|_{\lambda=0} \int_{\partial(\eta_X^\lambda(U_X))} j^3(\phi^\lambda \circ (\phi_X^\lambda)^{-1})^* [j^3(w \circ \phi^\lambda) \lrcorner \Theta_{\mathcal{L}}] \\
&= \left. \frac{d}{d\lambda} \right|_{\lambda=0} \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* j^3(\eta_Y^\lambda)^* [j^3(W) \lrcorner \Theta_{\mathcal{L}}] \\
&= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* \mathfrak{L}_{j^3(V)}(j^3(W) \lrcorner \Theta_{\mathcal{L}}) \\
&= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* d[j^3(V) \lrcorner j^3(W) \lrcorner \Theta_{\mathcal{L}}] \\
&\quad + \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner d(j^3(W) \lrcorner \Theta_{\mathcal{L}})],
\end{aligned}$$

where the last equality was obtained using Cartan's formula. We have also used the fact that $W^\lambda = w \circ \phi^\lambda$ and $W = w \circ \phi$ have the same k th prolongation. Furthermore, using Stoke's theorem, noting that $\partial\partial U_X$ is empty, and applying Cartan's formula once again to $d(j^3(W) \lrcorner \Theta_{\mathcal{L}})$, we obtain that

$$\begin{aligned}
d(\alpha_2(\mathcal{W}))(\phi) \cdot V &= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \mathfrak{L}_{j^3(W)} \Theta_{\mathcal{L}}] \\
&\quad - \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner j^3(W) \lrcorner \Omega_{\mathcal{L}}]. \tag{2.33}
\end{aligned}$$

Similarly,

$$\begin{aligned}
d(\alpha_2(\mathcal{V}))(\phi) \cdot W &= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(W) \lrcorner \mathfrak{L}_{j^3(V)} \Theta_{\mathcal{L}}] \\
&\quad - \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(W) \lrcorner j^3(V) \lrcorner \Omega_{\mathcal{L}}]. \tag{2.34}
\end{aligned}$$

Now, $j^3([V, W]) = [j^3(V), j^3(W)]$; hence,

$$\alpha_2(\phi) \cdot [V, W] = \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* ([j^3(V), j^3(W)] \lrcorner \Theta_{\mathcal{L}}).$$

Recall that for a differential form α on a manifold M and for vector fields X, Y on M ,

$$\mathbf{i}_{[X, Y]} \alpha = \mathfrak{L}_X \mathbf{i}_Y \alpha - \mathbf{i}_Y \mathfrak{L}_X \alpha.$$

Therefore,

$$\begin{aligned}
\alpha_2(\phi) \cdot [V, W] &= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [\mathfrak{L}_{j^3(V)}(j^3(W) \lrcorner \Theta_{\mathcal{L}}) - j^3(W) \lrcorner \mathfrak{L}_{j^3(V)} \Theta_{\mathcal{L}}] \\
&= \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(V) \lrcorner \mathfrak{L}_{j^3(W)} \Theta_{\mathcal{L}} - j^3(V) \lrcorner j^3(W) \lrcorner \Omega_{\mathcal{L}} \\
&\quad - j^3(W) \lrcorner \mathfrak{L}_{j^3(V)} \Theta_{\mathcal{L}}], \tag{2.35}
\end{aligned}$$

where we have again used Stoke’s theorem and Cartan’s formula twice. Substituting (2.33)–(2.35) into (2.31), we obtain that

$$d\alpha_2(\phi)(V, W) = \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(W) \lrcorner j^3(V) \lrcorner \Omega_{\mathcal{L}}]. \tag{2.36}$$

We now compute (2.32). Similar computations as above yield

$$d(\alpha_1(\mathcal{W}))(\phi) \cdot V = \int_{U_X} j^3(\phi \circ \phi_X^{-1})^* \mathfrak{L}_{j^3(V)}(j^3(W) \lrcorner \Omega_{\mathcal{L}}),$$

which vanishes for all $\phi \in \mathcal{P}$ and $V \in \mathcal{F}$. Similarly, $d(\alpha_1(\mathcal{V}))(\phi) \cdot W = 0$ for all $\phi \in \mathcal{P}$ and $W \in \mathcal{F}$. Finally, $\alpha_1(\phi) = 0$ for all $\phi \in \mathcal{P}$. Therefore, Eq. (2.32) vanishes for all $\phi \in \mathcal{P}$ and $V, W \in \mathcal{F}$. Using the latter and (2.36), Eq. (2.29) becomes

$$\int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(W) \lrcorner j^3(V) \lrcorner \Omega_{\mathcal{L}}] = 0$$

for all $\phi \in \mathcal{P}$ and all $V, W \in \mathcal{F}$, as desired. □

2.4. Noether’s theorem

Suppose that \mathcal{S} is invariant under the action $\Phi(g, \phi)$ of a Lie group G on \mathcal{C} . This implies that for each $g \in G$, $\Phi(g, \phi) \in \mathcal{P}$ whenever $\phi \in \mathcal{P}$. We restrict the action to elements of \mathcal{P} . For each element ξ of the Lie algebra \mathfrak{g} of G , let $\xi_{\mathcal{C}}$ be the corresponding infinitesimal generator on \mathcal{C} restricted to elements of \mathcal{P} . By the invariance of \mathcal{S} ,

$$\mathcal{S}(\Phi(\exp(t\xi), \phi)) = \mathcal{S}(\phi) \quad \forall t.$$

Differentiating with respect to t at $t = 0$, and using the fundamental property of the Cartan form that $\mathcal{L} \circ j^2(\phi \circ \phi_X^{-1}) = j^3(\phi \circ \phi_X^{-1})^* \Theta_{\mathcal{L}}$, we find that

$$\int_{U_X} j^3(\phi \circ \phi_X^{-1})^* \mathfrak{L}_{j^3(\xi_{\mathcal{C}}(\phi))} \Theta_{\mathcal{L}} = 0.$$

Then by Theorem 2.1 and the invariance of \mathcal{S} we have that

$$\begin{aligned} 0 &= (\xi_{\mathcal{C}} \lrcorner d\mathcal{S})(\phi) = \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(\xi_{\mathcal{C}}(\phi)) \lrcorner \Theta_{\mathcal{L}}] \\ &= - \int_{U_X} j^3(\phi \circ \phi_X^{-1})^* [j^3(\xi_{\mathcal{C}}(\phi)) \lrcorner \Omega_{\mathcal{L}}]. \end{aligned} \tag{2.37}$$

Definition 2.12. Let $J \in \text{Hom}(\mathfrak{g}, T^*\mathcal{C} \otimes \Lambda^n(J^3Y))$ satisfy

$$j^3(\xi_{\mathcal{C}}(\phi)) \lrcorner \Omega_{\mathcal{L}} = d[J(\xi)(\phi)] \tag{2.38}$$

for all $\xi \in \mathfrak{g}$ and $\phi \in \mathcal{C}$. Then the map $\mathbb{J} : \mathcal{C} \rightarrow \mathfrak{g}^*$ defined by

$$\langle \mathbb{J}(\phi), \xi \rangle = J(\xi)(\phi) \quad \forall \xi \in \mathfrak{g}, \phi \in \mathcal{C}, \tag{2.39}$$

is the *covariant momentum map of the action*.

With this definition, (2.37) becomes $\int_{U_X} d[j^3(\phi \circ \phi_X^{-1})^* \langle \mathbb{J}(\phi), \xi \rangle] = 0$, and since this holds for any $U_X \subset X$, the integrand must also vanish; thus,

$$d[j^3(\phi \circ \phi_X^{-1})^* \langle \mathbb{J}(\phi), \xi \rangle] = 0. \quad (2.40)$$

On the other hand, by Stoke's theorem we may also conclude that

$$\int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^* \langle \mathbb{J}(\phi), \xi \rangle = 0. \quad (2.41)$$

Last two statements are equivalent, and we refer to them as the covariant Noether's theorem.

3. A multisymplectic approach to the CH equation

3.1. CH equation

The completely integrable bi-Hamiltonian CH equation (see [2,4])

$$u_t - u_{yyt} = -3uu_y + 2u_y u_{yy} + uu_{yyy} \quad (3.1)$$

is a model for breaking shallow water waves that admits peaked solitary traveling waves as solutions (see [2,3]). Such solutions, termed *peakons*, develop from any initial data with sufficiently negative slope, and because of the discontinuities in the first derivative, these solutions are difficult to numerically simulate, particularly in the case of a *peakon-antipeakon collision* (see [3]).

The multisymplectic framework for the CH equation is intended to provide a foundation for numerical discretization schemes that preserve the Hamiltonian structure of this model, even at the discrete level. After developing the multisymplectic framework for (3.1), we shall follow [12] and develop the entire discrete multisymplectic approach to second-order field theories, concentrating on the discrete CH equation as our model problem. Although we shall only produce the simplest *multisymplectic-momentum* conserving algorithm for this equation, our construction is completely general and will allow for the creation of k th-order accurate schemes for arbitrarily large k .

The CH equation (3.1) is usually expressed in terms of the Eulerian, or spatial velocity field $u(t, y)$, and is the Euler-Poincaré equation for the reduced Lagrangian

$$l(u) = \frac{1}{2} \int (u^2 + u_y^2) dy. \quad (3.2)$$

Alternatively, one may express (3.1) in terms of the Lagrangian variable $\eta(t, x)$ arising from the solution of

$$\frac{\partial}{\partial t} \eta(x, t) = u(t, \eta(x, t)). \quad (3.3)$$

The Lagrangian approach to the CH equation is ideally suited to the multisymplectic variational theory, and we begin by specifying our fiber bundle $\pi_{XY} : Y \rightarrow X$. Let $X = S^1 \times \mathbb{R}$,

and $Y = S^1 \times \mathbb{R} \times \mathbb{R}$. We coordinatize X by (x^1, x^0) (or (x, t)) and Y by (x^1, x^0, y) (or (x, t, y)). A smooth section $\phi \in C^\infty(Y)$ represents a physical field and is expressed in local coordinates by $(x, t, \eta(x, t))$, where η is the Lagrangian flow solving (3.3). The material or Lagrangian velocity $(\partial/\partial t)\eta(x, t)$ is an element of $T_{\phi(x,t)}Y = T_{(x,t,y)}Y$, where $y = \eta(x, t)$.

Using (3.3) together with $u_y = \eta_{tx}/\eta_x$, the Lagrangian representation for the action may be expressed as

$$\mathcal{S}(\phi) = \frac{1}{2} \int_X (\eta_x \eta_t^2 + \eta_x^{-1} \eta_{tx}^2) dx dt. \tag{3.4}$$

The second jet bundle J^2Y is a nine-dimensional manifold and two-holonomic sections of $J^2Y \rightarrow X$ have local coordinates

$$j^2(\phi) = (x, t, \eta(x, t), \eta_x(x, t), \eta_t(x, t), \eta_{xx}(x, t), \eta_{xt}(x, t), \eta_{tx}(x, t), \eta_{tt}(x, t)),$$

where for smooth sections $\eta_{xt}(x, t) = \eta_{tx}(x, t)$. The Lagrangian density $\mathcal{L} : J^2Y \rightarrow \Lambda^2(X)$ is expressed as

$$\begin{aligned} \mathcal{L}(x^1, x^0, y, y_1, y_0, y_{11}, y_{10}, y_{01}, y_{00}) \\ = L(x^1, x^0, y, y_1, y_0, y_{11}, y_{10}, y_{01}, y_{00}) dx^1 \wedge dx^0. \end{aligned}$$

For the CH equation the Lagrangian density evaluated along the second jet of a section ϕ is given by

$$\mathcal{L}(j^2(\phi)) = [\frac{1}{2}(\eta_x \eta_t^2 + \eta_x^{-1} \eta_{tx}^2)] dx \wedge dt. \tag{3.5}$$

As our Lagrangian (3.5) depends only on y_1, y_0 , and y_{01} , the Euler–Lagrange equation (2.14) simply becomes

$$-\frac{\partial}{\partial x} \left(\frac{\partial L}{\partial \eta_x} \right) - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \eta_t} \right) + \frac{\partial^2}{\partial t \partial x} \left(\frac{\partial L}{\partial \eta_{tx}} \right) = 0, \tag{3.6}$$

so that we have the Lagrangian version of the CH equation (3.1) given by

$$\frac{1}{2} \left(\left(\frac{\eta_{tx}}{\eta_x} \right)^2 - \eta_t^2 \right)_x - (\eta_x \eta_t)_t + \left(\frac{\eta_{tx}}{\eta_x} \right)_{xt} = 0. \tag{3.7}$$

By differentiating $u = (\partial/\partial t)\eta \circ \eta^{-1}$ three times, one may verify that (3.7) is indeed equivalent to (3.1).

Now, using (2.11) we have that the Cartan form $\Theta_{\mathcal{L}}$ is given by

$$\begin{aligned} \Theta_{\mathcal{L}} = \frac{\partial L}{\partial \eta_x} d\eta \wedge dt - \left(\frac{\partial L}{\partial \eta_t} - D_x \left(\frac{\partial L}{\partial \eta_{tx}} \right) \right) d\eta \wedge dx + \frac{\partial L}{\partial \eta_{tx}} d\eta_t \wedge dt \\ + \left(L - \frac{\partial L}{\partial \eta_x} \eta_x - \frac{\partial L}{\partial \eta_t} \eta_t - \frac{\partial L}{\partial \eta_{tx}} \eta_{tx} + D_x \left(\frac{\partial L}{\partial \eta_{tx}} \right) \eta_t \right) dx \wedge dt, \end{aligned} \tag{3.8}$$

or

$$\begin{aligned} \Theta_{\mathcal{L}} = & \frac{\partial L}{\partial \eta_x} (d\eta \wedge dt - \eta_x dx \wedge dt) + \left(\frac{\partial L}{\partial \eta_t} - D_x \left(\frac{\partial L}{\partial \eta_{tx}} \right) \right) (-d\eta \wedge dx - \eta_t dx \wedge dt) \\ & + \frac{\partial L}{\partial \eta_{tx}} (d\eta_t \wedge dt - \eta_{tx} dx \wedge dt) + L dx \wedge dt, \end{aligned} \quad (3.9)$$

if written in terms of the system of contact forms.

3.2. Multisymplectic form formula for the CH equation

Marsden et al. [12] in their paper have demonstrated how the multisymplectic form formula for first-order field theories when applied to nonlinear wave equations generalizes the notion of symplecticity given by Bridges in [1]. Using the example of the CH equation, we present below a simple interpretation of the multisymplectic form formula for the second-order field theories. We show that the MFF formula is an intrinsic generalization of the conservation law analogous to the one in Appendix D of [1].

Bridges has introduced the notion of a Hamiltonian system on a multisymplectic structure. A multisymplectic structure $(\mathcal{M}, \omega^1, \dots, \omega^n, \omega^0)$ consists of a manifold \mathcal{M} , the phase space, and a family of pre-symplectic forms. The phase space \mathcal{M} is a manifold modeled on \mathbb{R}^{n+1} . A Hamiltonian system on a multisymplectic structure is then represented symbolically by $(\mathcal{M}, \omega^1, \dots, \omega^n, \omega^0, H)$ with the governing equation

$$\omega^1 \left(\frac{\partial Z}{\partial x^1}, v \right) + \dots + \omega^n \left(\frac{\partial Z}{\partial x^n}, v \right) + \omega^0 \left(\frac{\partial Z}{\partial t}, v \right) = \langle \nabla H(Z), v \rangle \quad (3.10)$$

for all vector fields v on \mathcal{M} where $\langle \cdot, \cdot \rangle$ is an inner product on $T\mathcal{M}$ and $Z(x^1, \dots, x^n, t)$ is a curve in \mathcal{M} . Bridges has shown that this formulation is natural for studying wave propagation in open systems. Bridges, in particular, has obtained the following conservation law in the case of the wave equation [1]:

$$\frac{\partial}{\partial t} \omega^0(Z_t, Z_x) + \frac{\partial}{\partial x} \omega^1(Z_t, Z_x) = 0. \quad (3.11)$$

This law generalizes the notion of symplecticity of classical mechanics.

Let us make an appropriate choice of the phase space \mathcal{M} for the CH equation. Our choice is entirely governed by the coefficients in the Cartan form (3.8). Since the Lagrangian (3.5) does not explicitly depend on time and space variables, i.e., the system is autonomous, we identify sections ϕ of Y with mappings $\eta(x, t)$ from \mathbb{R}^2 into \mathbb{R} , and similarly, sections of J^3Y with mappings from \mathbb{R}^2 into \mathbb{R}^{15} . The Cartan form (3.8) suggests to introduce the following momenta:

$$p^x = \frac{\partial L}{\partial \eta_x}, \quad p^t = \frac{\partial L}{\partial \eta_t} - D_x \left(\frac{\partial L}{\partial \eta_{tx}} \right), \quad p^{tx} = \frac{\partial L}{\partial \eta_{tx}}, \quad p^{xx} = p^{tt} = p^{xt} = 0. \quad (3.12)$$

Since $\Theta_{\mathcal{L}}$ is horizontal over J^1Y , the covariant configuration bundle is really $J^1Y \rightarrow X$, and one should think of (η, η_x, η_t) as field variables with each field variable having conjugate

multi-momenta. For example, p^x, p^t function as conjugate spatial and temporal momenta for the field component η . Then the transformation

$$(\eta, \eta_x, \eta_t, \eta_{xx}, \eta_{xt}, \eta_{tx}, \eta_{tt}, \dots) \mapsto (\eta, \eta_x, \eta_t, p^x, p^t, p^{tx})$$

defines a mapping from the space of vertical sections of $J^3Y \rightarrow X$ into the phase space $\mathcal{M} = \mathbb{R}^6$ modeled over $X = \mathbb{R}^2$. We denote this transformation by $\mathbb{F}L$. Let us now state the result that connects our paper to Bridges’ theory.

Proposition 3.1. *The multisymplectic form formula (MFF) yields a multisymplectic structure $(\mathcal{M}, \omega^1, \omega^0)$ such that the MFF formula becomes an intrinsic generalization of the following conservation law: for any V, W in \mathcal{F} that are π_{XY} -vertical,*

$$\frac{\partial}{\partial x} \omega^1(T\mathbb{F}L \cdot j^3(V), T\mathbb{F}L \cdot j^3(W)) + \frac{\partial}{\partial t} \omega^0(T\mathbb{F}L \cdot j^3(V), T\mathbb{F}L \cdot j^3(W)) = 0. \tag{3.13}$$

Moreover, the CH equation in both Eulerian form(3.1) and Lagrangian form(3.7) is equivalent to the Hamiltonian system of equations on the multisymplectic structure with the Hamiltonian defined by

$$H = L - p^x \eta_x - p^t \eta_t - p^{tx} \eta_{tx}. \tag{3.14}$$

Proof. Consider two π_{XY} -vertical vectors V and W in \mathcal{F} . Then $T\mathbb{F}L \cdot j^3(V)$ and $T\mathbb{F}L \cdot j^3(W)$ are vertical-over- X vector fields on $X \times \mathcal{M} \rightarrow X$, whose components we shall denote via

$$(V^\eta, V^{\eta_x}, V^{\eta_t}, V^{p^x}, V^{p^t}, V^{p^{tx}}),$$

or just numerate by $(V^1, V^2, V^3, V^4, V^5, V^6)$. Thinking of the components of the transformation $\mathbb{F}L$ as functions on J^3Y , we immediately see that

$$\begin{aligned} V^{p^x} &= dp^x \cdot j^3(V) \equiv j^3(V)[p^x], \\ V^{p^t} &= dp^t \cdot j^3(V) \equiv j^3(V)[p^t], \\ V^{p^{tx}} &= dp^{tx} \cdot j^3(V) \equiv j^3(V)[p^{tx}]. \end{aligned} \tag{3.15}$$

Using expressions (3.12) we express $\Omega_{\mathcal{L}}$ as

$$\begin{aligned} \Omega_{\mathcal{L}} &= dp^x \wedge d\eta \wedge dt - dp^t \wedge d\eta \wedge dx + dp^{tx} \wedge d\eta_t \wedge dt \\ &\quad - \eta_x dp^x \wedge dx \wedge dt - \eta_t dp^t \wedge dx \wedge dt - \eta_{tx} dp^{tx} \wedge dx \wedge dt. \end{aligned}$$

Next, combining with (3.15) we obtain that

$$\begin{aligned} j^3(W) \lrcorner j^3(V) \lrcorner \Omega_{\mathcal{L}} &= \{V^{p^x} W^\eta - W^{p^x} V^\eta + V^{p^{tx}} W^{\eta_t} - W^{p^{tx}} V^{\eta_t}\} dt \\ &\quad - \{V^{p^t} W^\eta - W^{p^t} V^\eta\} dx, \end{aligned}$$

so that

$$\begin{aligned} & \int_{\partial U_X} j^3(\phi \circ \phi_X^{-1})^*[j^3(W) \lrcorner j^3(V) \lrcorner \Omega_{\mathcal{L}}] \\ &= \int_{\partial U_X} (V^4 W^1 - W^4 V^1 + V^6 W^3 - W^6 V^3) dt \\ & \quad - (V^5 W^1 - W^5 V^1) dx. \end{aligned} \tag{3.16}$$

The integral on the right-hand side of the above equation leads us to introduce two degenerate skew-symmetric matrices B_1, B_0 on \mathbb{R}^6 :

$$B_1 = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \end{bmatrix}, \quad B_0 = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

To each matrix B_ν , we associate the 2-form ω^ν on \mathbb{R}^6 given by $\omega^\nu(u, v) = \langle B_\nu u, v \rangle \equiv v^T B_\nu u$, where $u, v \in \mathbb{R}^6$. With the definition of ω^ν and the use of (3.16), the multisymplectic form formula (2.27) becomes, for $U_X \subset X$,

$$\int_{\partial U_X} \omega^1(T\mathbb{F}L \cdot j^3(V), T\mathbb{F}L \cdot j^3(W)) dt - \omega^0(T\mathbb{F}L \cdot j^3(V), T\mathbb{F}L \cdot j^3(W)) = 0.$$

Hence by the Stoke’s theorem,

$$\begin{aligned} & \int_{\partial U_X} \left[\frac{\partial}{\partial x} \omega^1(T\mathbb{F}L \cdot j^3(V), T\mathbb{F}L \cdot j^3(W)) \right. \\ & \left. + \frac{\partial}{\partial t} \omega^0(T\mathbb{F}L \cdot j^3(V), T\mathbb{F}L \cdot j^3(W)) \right] dx \wedge dt = 0. \end{aligned}$$

Since U_X is arbitrary, we obtain the desired conservation law (3.13).

In the special case, when the components $V^\eta = \eta_x$ and $W^\eta = \eta_t$, one may verify that

$$\begin{aligned} T\mathbb{F}L \cdot j^3(V) &= (\eta, \eta_x, \eta_t, p^x, p^t, p^{tx})_{,x}, \\ T\mathbb{F}L \cdot j^3(W) &= (\eta, \eta_x, \eta_t, p^x, p^t, p^{tx})_{,t}, \end{aligned}$$

so that, letting Z denote an element $(\eta, \eta_x, \eta_t, p^x, p^t, p^{tx}) \in \mathcal{M}$, the formula (3.11) takes the special form

$$\frac{\partial}{\partial x} \omega^1(Z_t, Z_x) + \frac{\partial}{\partial t} \omega^0(Z_t, Z_x) = 0,$$

which is the complete analog of Bridges’ conservation law (3.11) for the wave equation.

Next, since the inner product $\langle \cdot, \cdot \rangle$ is independent of $Z \in \mathcal{M}$, the Hamiltonian system of equations (3.10) on the multisymplectic structure $(\mathcal{M}, \omega^1, \omega^0)$ may be written as

$$Z_x \lrcorner \omega^1 + Z_t \lrcorner \omega^0 = \nabla H, \quad B_1 Z_x + B_0 Z_t = \nabla H,$$

which results in

$$\begin{aligned} \frac{\partial}{\partial x} p^x + \frac{\partial}{\partial t} p^t &= \frac{\partial H}{\partial \eta}, & \frac{\partial}{\partial x} p^{tx} &= \frac{\partial H}{\partial \eta_t}, & \frac{\partial}{\partial x} \eta &= -\frac{\partial H}{\partial p^x}, \\ \frac{\partial}{\partial t} \eta &= -\frac{\partial H}{\partial p^t}, & \frac{\partial}{\partial x} \eta_t &= -\frac{\partial H}{\partial p^{tx}}. \end{aligned}$$

With the choice of the Hamiltonian (3.14) the last four equations yield identities, and the first equation becomes

$$\frac{\partial}{\partial x} p^x + \frac{\partial}{\partial t} p^t = 0.$$

Using the Legendre transformation expressions (3.12) for p^x, p^t , the latter equation recovers the Euler–Lagrange equation (3.6), and hence (3.7). In other words, the Euler–Lagrange equations on J^3Y are equivalent to Hamilton’s equations on the multisymplectic structure $(\mathcal{M}, \omega^1, \omega^0, H)$. \square

4. Discrete second-order multisymplectic field theory

4.1. A general construction

We shall now generalize the Veselov-type discretization of first-order field theory given in [12] to second-order field theories, using the CH equation as our example. We discretize X by $\mathbb{Z} \times \mathbb{Z} = \{(i, j)\}$ and the fiber bundle Y by $X \times \mathbb{R}$. Elements of Y over the base point (i, j) are written as y_{ij} and the projection π_{XY} acts on Y by $\pi_{XY}(y_{ij}) = (i, j)$. The fiber over $(i, j) \in X$ is denoted by Y_{ij} .

For the general case of a second-order Lagrangian one must define the discrete second jet bundle of Y , and this discretization depends on how one chooses to approximate the partial derivatives of the field. For example, using central differencing and a fixed time step k and space step h , we have that

$$\begin{aligned} \eta_x &\approx \frac{y_{i+1j} - y_{i-1j}}{2h}, & \eta_t &\approx \frac{y_{ij+1} - y_{ij-1}}{2k}, & \eta_{xx} &\approx \frac{y_{i-1j} - 2y_{ij} + y_{i+1j}}{h^2}, \\ \eta_{tx} &\approx \frac{y_{i+1j+1} - y_{i+1j-1} + y_{i-1j-1} - y_{i-1j+1}}{4hk}, & \eta_{tt} &\approx \frac{y_{ij-1} - 2y_{ij} + y_{ij+1}}{k^2}, \end{aligned} \tag{4.1}$$

where $y_{ij} = \eta(x_i, t_j)$ and $\{(x_i, t_j)\}$ form a uniform grid in continuous space–time (Fig. 1).

We observe that a 9-tuple

$$(y_{i-1j-1}, y_{i-1j}, y_{i-1j+1}, y_{ij-1}, y_{ij}, y_{ij+1}, y_{i+1j-1}, y_{i+1j}, y_{i+1j+1})$$

is sufficient to approximate $j^2\phi(P)$, where P is in the center of the cell

$$\begin{aligned} \boxplus_{ij} &\equiv ((i-1, j-1), (i-1, j), (i-1, j+1), (i, j-1), \\ &(i, j), (i, j+1), (i+1, j-1), (i+1, j), (i+1, j+1)). \end{aligned}$$

Let X^{\boxplus} denote the set of cells, i.e., $X^{\boxplus} = \{\boxplus_{ij} | (i, j) \in X\}$. Components of a cell are called vertices, and are numbered from first to ninth. A point $(i, j) \in X$ is touched by a cell if it

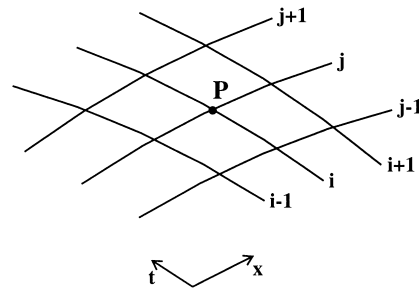


Fig. 1. Equivalent computational grid in the physical domain.

is a vertex of that cell. If $U \subseteq V$, then $(i, j) \in X$ is an *interior point* of U if U contains all cells touching (i, j) . The *interior* $\text{int } U$ of U is the set of all interior points of U . The *closure* $\text{cl } U$ of U is the union of all cells touching interior points of U . A *boundary point* of U is a point in U and $\text{cl } U$ which is not an interior point. The *boundary* of U is the set of boundary points, so that $\partial U \equiv (U \cap \text{cl } U) \setminus \text{int } U$.

A *section* of the configuration bundle $Y \rightarrow X$ is a map $\phi : U \subseteq X \rightarrow Y$ such that $\pi_{XY} \circ \phi = \text{id}_U$. We are now ready to define the discrete multisymplectic phase space.

Definition 4.1. The discrete *second jet bundle* of Y is given by

$$J^2Y \equiv \{(y_{i-1j-1}, y_{i-1j}, y_{i-1j+1}, y_{ij-1}, y_{ij}, y_{ij+1}, y_{i+1j-1}, y_{i+1j}, y_{i+1j+1}) | (i, j) \in X, y_{i-1j-1}, \dots, y_{i+1j+1} \in \mathbb{R}\} \equiv X^{\boxplus} \times \mathbb{R}^9.$$

The fiber over $(i, j) \in X$ is denoted J^2Y_{ij} . We define the *second jet extension* of a section ϕ to be the map $j^2\phi : X \rightarrow J^2Y$ given by

$$j^2\phi(i, j) \equiv (\boxplus_{ij}, \phi(i-1, j-1), \phi(i-1, j), \phi(i-1, j+1), \phi(i, j-1), \phi(i, j), \phi(i, j+1), \phi(i+1, j-1), \phi(i+1, j), \phi(i+1, j+1)).$$

Given a vector field v on Y the *second jet extension* of v is the vector field j^2v on J^2Y defined by

$$j^2v(y_{i-1j-1}, \dots, y_{i+1j+1}) \equiv (v(y_{i-1j-1}), v(y_{i-1j}), v(y_{i-1j+1}), v(y_{ij-1}), v(y_{ij}), v(y_{ij+1}), v(y_{i+1j-1}), v(y_{i+1j}), v(y_{i+1j+1})).$$

Of course, this may easily be generalized to more accurate differencing schemes that require more than nine grid points to define second partial derivatives.

4.2. A multisymplectic-momentum algorithm for the CH equation

Restricting our attention to the CH equation and noting that its Lagrangian depends only on $\eta_x, \eta_t, \eta_{tx}$, we may significantly simplify our discretization of the second jet bundle J^2Y ; this will substantially reduce our calculations and simplify the exposition.

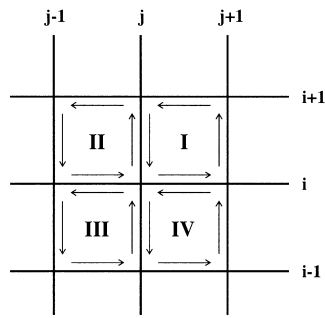


Fig. 2. The rectangles which touch (i, j) .

To approximate $j^2\phi(P)$ we choose the forward difference evaluations of $\eta_x, \eta_t, \eta_{tx}$:

$$\eta_x \approx \frac{y_{i+1j} - y_{ij}}{h}, \quad \eta_t \approx \frac{y_{ij+1} - y_{ij}}{k}, \quad \eta_{tx} \approx \frac{y_{i+1j+1} - y_{i+1j} - y_{ij+1} + y_{ij}}{hk}.$$

For this particular choice, our cell reduces to a rectangle. A *rectangle* \square of X is an ordered 4-tuple of the form

$$\square_{ij} = ((i, j), (i + 1, j), (i + 1, j + 1), (i, j + 1)).$$

For each rectangle, $\square^1, \square^2, \square^3,$ and \square^4 stand for the first, second, third, and fourth vertices, respectively. If (i, j) is the first vertex, we shall denote the rectangle by \square_{ij} . The set of all rectangles in X is denoted by X^\square . The set-theoretical definitions of Section 4.1 apply here. For example, a point $P = (i, j) \in X$ is *touched* (see Fig. 2) by four rectangles $\square_{ij}, \square_{i-1j}, \square_{i-1j-1}, \square_{ij-1}$, etc.

Again as (3.5) does not depend on η_{xx}, η_{tt} , we may restrict ourselves to a subbundle $\tilde{\mathcal{B}}$ of the continuous J^2Y defined via $\tilde{\mathcal{B}} \equiv \{s \in J^2Y | s_{\mu\mu} = 0 \text{ for } \mu = 1, 0\}$. Then the discrete analog \mathcal{B} (see Fig. 3) of $\tilde{\mathcal{B}}$ is identified with

$$\begin{aligned} \tilde{\mathcal{B}} &\equiv \{(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) | (i, j) \in X, y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1} \in \mathbb{R}\} \\ &\equiv X^\square \times \mathbb{R}^4. \end{aligned}$$

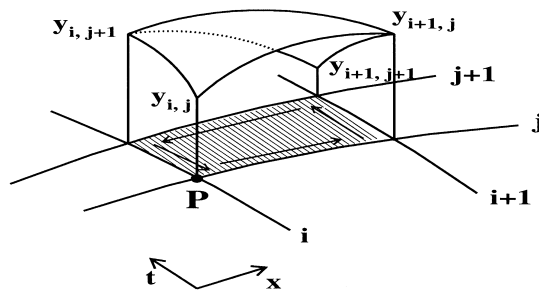


Fig. 3. Interpretation of an element of J^2Y when X is discrete.

For a section $\phi : U \subseteq X \rightarrow Y$, we define the *second jet extension* of ϕ to \mathcal{B} to be the map $j^2\phi : U \subseteq X \rightarrow \mathcal{B}$ via

$$j^2\phi(i, j) = (\square_{ij}, \phi(\square^1), \phi(\square^2), \phi(\square^3), \phi(\square^4)).$$

Given a vector field v on Y we extend it to a vector field j^2v on \mathcal{B} by

$$j^2v(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) = (v(y_{ij}), v(y_{i+1j}), v(y_{i+1j+1}), v(y_{ij+1})).$$

A *discrete Lagrangian* on \mathcal{B} is then a function $L : \mathcal{B} \rightarrow \mathbb{R}$ of five variables $\square_{ij}, y_1, y_2, y_3, y_4$, where the y -variables are labeled in the order they appear in a 4-tuple. Let U be a *regular* subset of X , i.e., U is exactly the union of its interior and boundary. Let \mathcal{C}_U denote the set of sections of Y on U , so \mathcal{C}_U is the manifold $\mathbb{R}^{|U|}$.

Definition 4.2. The *discrete action* is a real valued function on \mathcal{C}_U defined by the rule

$$\mathcal{S}(\phi) \equiv \sum_{\square \subseteq U; (i,j) = \square^1} L \circ j^2\phi(i, j). \tag{4.2}$$

Given a section ϕ on U acting as $\phi(i, j) = y_{ij}$, one can define an element $V \in T_\phi\mathcal{C}_U$ to be a map $V : U \rightarrow TY$ acting as $V(i, j) = (\phi(i, j), v_{ij})$, where v_{ij} is thought as a vector emanating from $y_{ij} = \phi(i, j)$. Given an element $V \in T_\phi\mathcal{C}_U$ one can always extend it to a vector field v on Y . On the other hand, given a vector field v on Y , $V \equiv v \circ \phi$ is an element of $T_\phi\mathcal{C}_U$. Thus, it is sufficient to work with vector fields v on Y alone.

If v is a vector field on Y , consider its restriction $v|_{Y_{ij}}$ to the fiber Y_{ij} . Let $F_\lambda^v : Y_{ij} \rightarrow Y_{ij}$ be the flow of $v|_{Y_{ij}}$. Then by definition of the flow,

$$v(\phi(i, j)) = \left. \frac{d}{d\lambda} \right|_{\lambda=0} F_\lambda^v(\phi(i, j)).$$

Therefore, there is the 1-parameter family of sections on U defined by $\phi^\lambda \equiv F_\lambda^v \circ \phi$ such that $\phi^0 = \phi$ and $(d/d\lambda)|_{\lambda=0} \phi^\lambda = v \circ \phi = V$. Thus, the *variational principle* is to seek those sections ϕ for which

$$\left. \frac{d}{d\lambda} \right|_{\lambda=0} \mathcal{S}(F_\lambda^v \circ \phi) = 0 \tag{4.3}$$

for all vector fields v on Y .

4.3. Discrete Euler–Lagrange equations

With our choice of \mathcal{B} , the discrete Lagrangian for the CH equation is

$$L(y_1, y_2, y_3, y_4) = \frac{1}{2} \left(\frac{y_2 - y_1}{h} \frac{(y_4 - y_1)^2}{k^2} + \frac{h}{y_2 - y_1} \frac{(y_3 - y_2 - y_4 + y_1)^2}{h^2 k^2} \right). \tag{4.4}$$

The variational principle yields the *discrete Euler–Lagrange field equations* (DEL equations) as follows. Choose an arbitrary point $(i, j) \in U$. Henceforth, with a slight abuse

of notation, we shall write y_{ij} for $\phi(i, j)$. The action (4.2), written with its summands containing y_{ij} explicitly, is (see Figs. 2, 3)

$$\mathcal{S} = \cdots + L(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) + L(y_{i-1j}, y_{ij}, y_{ij+1}, y_{i-1j+1}) \\ + L(y_{i-1j-1}, y_{ij-1}, y_{ij}, y_{i-1j}) + L(y_{ij-1}, y_{i+1j-1}, y_{i+1j}, y_{ij}) + \cdots .$$

Differentiating with respect to y_{ij} yields the DEL equations:

$$\frac{\partial L}{\partial y_1}(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \\ + \frac{\partial L}{\partial y_2}(y_{i-1j}, y_{ij}, y_{ij+1}, y_{i-1j+1}) \\ + \frac{\partial L}{\partial y_3}(y_{i-1j-1}, y_{ij-1}, y_{ij}, y_{i-1j}) + \frac{\partial L}{\partial y_4}(y_{ij-1}, y_{i+1j-1}, y_{i+1j}, y_{ij}) = 0$$

for all $(i, j) \in \text{int } U$. Equivalently, these equations may be written as

$$\sum_{l; \square; (i,j)=\square^l} \frac{\partial L}{\partial y_l}(\phi(\square^1), \phi(\square^2), \phi(\square^3), \phi(\square^4)) = 0 \tag{4.5}$$

for all $(i, j) \in \text{int } U$. Computing and evaluating $\partial L/\partial y_i$ along rectangles touching an interior point (i, j) , and substituting these expressions into (4.5), we obtain the discrete Euler–Lagrange equations for the CH equation:

$$\frac{(\Delta_k y_{i+1j} - \Delta_k y_{ij})^2}{2hk^2(\Delta_h y_{ij})^2} - \frac{(\Delta_k y_{ij} - \Delta_k y_{i-1j})^2}{2hk^2(\Delta_h y_{i-1j})^2} - \frac{(\Delta_k y_{ij})^2}{2hk^2} \\ + \frac{(\Delta_k y_{i-1j})^2}{2hk^2} + \frac{(\Delta_k y_{i+1j} - \Delta_k y_{ij})}{hk^2(\Delta_h y_{ij})} - \frac{(\Delta_k y_{ij} - \Delta_k y_{i-1j})}{hk^2(\Delta_h y_{i-1j})} \\ - \frac{(\Delta_k y_{i+1j-1} - \Delta_k y_{ij-1})}{hk^2(\Delta_h y_{ij-1})} + \frac{(\Delta_k y_{ij-1} - \Delta_k y_{i-1j-1})}{hk^2(\Delta_h y_{i-1j-1})} \\ - \frac{(\Delta_h y_{ij})(\Delta_k y_{ij})}{hk^2} + \frac{(\Delta_h y_{ij-1})(\Delta_k y_{ij-1})}{hk^2} = 0, \tag{4.6}$$

where

$$\Delta_k y_{ij} = y_{ij+1} - y_{ij}, \quad \Delta_k y_{i-1j} = y_{i-1j+1} - y_{i-1j}, \\ \Delta_h y_{ij} = y_{i+1j} - y_{ij}, \quad \Delta_k y_{i+1j} = y_{i+1j+1} - y_{i+1j}.$$

To see that (4.6) is indeed approximating the continuous Euler–Lagrange equation (3.7), notice that the first two terms combine to approximate

$$\frac{1}{2} \left(\left(\frac{\eta_{tx}}{\eta_x} \right)^2 \right)_x \approx \frac{1}{2} \frac{1}{h} \left[\frac{((\Delta_k y_{i+1j} - \Delta_k y_{ij})/hk)^2}{(\Delta_h y_{ij}/h)^2} - \frac{((\Delta_k y_{ij} - \Delta_k y_{i-1j})/hk)^2}{(\Delta_h y_{i-1j}/h)^2} \right].$$

As to the third and fourth terms of (4.6),

$$-\frac{1}{2}(\eta_t^2)_x \approx -\frac{1}{2} \frac{1}{h} \left[\left(\frac{\Delta_k y_{ij}}{k} \right)^2 - \left(\frac{\Delta_k y_{i-1j}}{k} \right)^2 \right].$$

Next, the fifth, sixth, seventh, and eighth terms combine as

$$\left(\frac{\eta_{tx}}{\eta_x}\right)_{tx} \approx \frac{1}{hk} \left[\left(\frac{((\Delta_k y_{i+1j} - \Delta_k y_{ij})/hk)}{(\Delta_h y_{ij}/h)} \right) - \left(\frac{((\Delta_k y_{ij} - \Delta_k y_{i-1j})/hk)}{(\Delta_h y_{i-1j}/h)} \right) \right. \\ \left. - \left(\frac{((\Delta_k y_{i+1j-1} - \Delta_k y_{ij-1})/hk)}{(\Delta_h y_{ij-1}/h)} \right) + \left(\frac{((\Delta_k y_{ij-1} - \Delta_k y_{i-1j-1})/hk)}{(\Delta_h y_{i-1j-1}/h)} \right) \right].$$

Finally, the last two terms of (4.6) approximate

$$-(\eta_x \eta_t)_t \approx -\frac{1}{k} \left(\frac{\Delta_h y_{ij}}{h} \frac{\Delta_k y_{ij}}{k} - \frac{\Delta_h y_{ij-1}}{h} \frac{\Delta_k y_{ij-1}}{k} \right).$$

The numerical scheme (4.6) proceeds as follows: suppose that

$$\Delta_h y_{ij}, \Delta_h y_{i-1j}, \Delta_h y_{i-1j-1}, \Delta_h y_{ij-1}, \Delta_k y_{ij-1}, \Delta_k y_{i-1j-1}, \Delta_k y_{i+1j-1}$$

as known from the two previous time steps; then (4.6) may be written as

$$\mathbf{F}(\Delta_k y_{ij}, \Delta_k y_{i+1j}, \Delta_k y_{i-1j}) = 0.$$

These are implicit equations which must be solved for y_{ij+1} , $1 \leq i \leq N$, where N is the size of the spatial grid.

4.4. Discrete Cartan form

We consider arbitrary variations which are in no way constrained on the boundary ∂U . For each $(i, j) \in \partial U$ there is at least one rectangle in U touching (i, j) since $(i, j) \in \text{cl } U$ and U is regular. On the other hand, not all four rectangles touching (i, j) are in U since $(i, j) \notin \text{int } U$. Therefore, each $(i, j) \in \partial U$ occurs as the l th vertex for either one, two, or three of the $l \in 1, 2, 3, 4$ and the corresponding l th boundary expressions are given by

$$\frac{\partial L}{\partial y_1}(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1})V(i, j), \quad \frac{\partial L}{\partial y_2}(y_{i-1j}, y_{ij}, y_{ij+1}, y_{i-1j+1})V(i, j), \\ \frac{\partial L}{\partial y_3}(y_{i-1j-1}, y_{ij-1}, y_{ij}, y_{i-1j})V(i, j), \quad \frac{\partial L}{\partial y_4}(y_{ij-1}, y_{i+1j-1}, y_{i+1j}, y_{ij})V(i, j),$$

(4.7)

where $y_{ij} = \phi(i, j)$. The sum of all such terms is the contribution to dS from the boundary ∂U . We thus define the four 1-forms on $\mathcal{B} \subseteq J^2 Y$ by

$$\Theta_L^1(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (v_{y_{ij}}, v_{y_{i+1j}}, v_{y_{i+1j+1}}, v_{y_{ij+1}}) \\ \equiv \frac{\partial L}{\partial y_1}(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (v_{y_{ij}}, 0, 0, 0), \\ \Theta_L^2(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (v_{y_{ij}}, v_{y_{i+1j}}, v_{y_{i+1j+1}}, v_{y_{ij+1}}) \\ \equiv \frac{\partial L}{\partial y_2}(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (0, v_{y_{i+1j}}, 0, 0),$$

$$\begin{aligned} &\Theta_L^3(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (v_{y_{ij}}, v_{y_{i+1j}}, v_{y_{i+1j+1}}, v_{y_{ij+1}}) \\ &\equiv \frac{\partial L}{\partial y_3}(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (0, 0, v_{y_{i+1j+1}}, 0), \end{aligned}$$

$$\begin{aligned} &\Theta_L^4(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (v_{y_{ij}}, v_{y_{i+1j}}, v_{y_{i+1j+1}}, v_{y_{ij+1}}) \\ &\equiv \frac{\partial L}{\partial y_4}(y_{ij}, y_{i+1j}, y_{i+1j+1}, y_{ij+1}) \cdot (0, 0, 0, v_{y_{ij+1}}). \end{aligned}$$

We regard the 4-tuple $(\Theta_L^1, \Theta_L^2, \Theta_L^3, \Theta_L^4)$ as being the discrete analog of the multisymplectic form $\Theta_{\mathcal{L}}$. Given a vector field v on Y such that $V = v \circ \phi$, the first expression from the list (4.7) becomes $[(j^2\phi)^*(j^2v \lrcorner \Theta_L^1)](i, j)$, the others written similarly. With this notation, $d\mathcal{S}$ may be expressed as

$$\begin{aligned} d\mathcal{S}(\phi) \cdot V = & \sum_{(i,j) \in \text{int } U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} [(j^2\phi)^*(j^2v \lrcorner \Theta_L^l)](\square^l) \right) \\ & + \sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} [(j^2\phi)^*(j^2v \lrcorner \Theta_L^l)](\square^l) \right). \end{aligned} \tag{4.8}$$

4.5. Discrete multisymplectic form formula

For a rectangle \square in X , define the projection $\pi_{\square} : \mathcal{C}_U \rightarrow \mathcal{B}$ by

$$\pi_{\square}(\phi) \equiv (\square, \phi(\square^1), \phi(\square^2), \phi(\square^3), \phi(\square^4)).$$

Calculating the form $\pi_{\square}^* \Theta_L^l$ on \mathcal{C}_U gives

$$(\pi_{\square}^* \Theta_L^l)(\phi) \cdot V = \frac{\partial L}{\partial y_l}(\phi(\square^1), \phi(\square^2), \phi(\square^3), \phi(\square^4)) V(\square^l).$$

This immediately implies that the variation (4.8) can be written as

$$\begin{aligned} d\mathcal{S}(\phi) \cdot V = & \sum_{(i,j) \in \text{int } U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} (\pi_{\square}^* \Theta_L^l)(\phi) \cdot V \right) \\ & + \sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} (\pi_{\square}^* \Theta_L^l)(\phi) \cdot V \right). \end{aligned} \tag{4.9}$$

Define the 1-forms α_1 and α_2 on the space of sections \mathcal{C}_U to be the first and the second terms on the right-hand side of (4.9), respectively.

As in Section 4.4 we would like to derive the discrete analog of symplecticity of the flow in mechanics. Let ϕ^λ be a curve of solutions of (4.5) that passes through ϕ at zero with $V = (d/d\lambda)|_{\lambda=0} \phi^\lambda$. Then for each interior point (i, j) and each λ , the following holds:

$$\sum_{l; \square; (i,j)=\square^l} \frac{\partial L}{\partial y_l} (\phi^\lambda(\square^1), \phi^\lambda(\square^2), \phi^\lambda(\square^3), \phi^\lambda(\square^4)) = 0.$$

Differentiating these equations with respect to λ at $\lambda = 0$, we obtain the following definition.

Definition 4.3. If ϕ is a solution of the discrete Euler–Lagrange equations (4.5), then a first-variation equation solution at ϕ is a vector $V \in T_\phi \mathcal{C}_U$ such that for each $(i, j) \in \text{int } U$,

$$\sum_{l; \square; (i,j)=\square^l} \sum_{k=1}^4 \frac{\partial^2 L}{\partial y_k \partial y_l} (\phi(\square^1), \phi(\square^2), \phi(\square^3), \phi(\square^4)) V(\square^k) = 0. \quad (4.10)$$

By definition of the forms α_1 and α_2 , $dS = \alpha_1 + \alpha_2$. Since $d^2S = 0$, $d\alpha_1 + d\alpha_2 = 0$. Using (4.9) and denoting the vertices of \square by y_1, y_2, y_3, y_4 , we have that $\Theta_L^l = (\partial L / \partial y_l) dy_l$, which implies that for all $l = 1, 2, 3, 4$,

$$\Omega_L^l = \sum_{k=1}^4 \frac{\partial^2 L}{\partial y_k \partial y_l} dy_k \wedge dy_l.$$

Therefore,

$$\begin{aligned} \pi_\square^* \Omega_L^l(\phi)(V, W) &= \Omega_L^l(\pi_\square(\phi))(T_\phi \pi_\square \cdot V, T_\phi \pi_\square \cdot W) \\ &= \Omega_L^l(\phi(\square^1) \cdots \phi(\square^4)) \cdot ((V(\square^1) \cdots V(\square^4)), (W(\square^1) \cdots W(\square^4))) \\ &= \sum_{k=1}^4 \frac{\partial^2 L}{\partial y_k \partial y_l} (\phi(\square^1), \phi(\square^2), \phi(\square^3), \phi(\square^4)) \{V(\square^k) W(\square^l) - V(\square^l) W(\square^k)\}. \end{aligned} \quad (4.11)$$

Substitution of (4.11) into the exterior derivative of the right-hand side of (4.9) yields

$$\begin{aligned} d\alpha_1(\phi)(V, W) &= \sum_{(i,j) \in \text{int } U} \\ &\left(\sum_{\square \subseteq U; l; (i,j)=\square^l} \sum_{k=1}^4 \frac{\partial^2 L}{\partial y_k \partial y_l} (\phi(\square^1) \cdots \phi(\square^4)) (V(\square^k) W(\square^l) - V(\square^l) W(\square^k)) \right), \\ d\alpha_2(\phi)(V, W) &= \sum_{(i,j) \in \partial U} \\ &\left(\sum_{\square \subseteq U; l; (i,j)=\square^l} \sum_{k=1}^4 \frac{\partial^2 L}{\partial y_k \partial y_l} (\phi(\square^1) \cdots \phi(\square^4)) (V(\square^k) W(\square^l) - V(\square^l) W(\square^k)) \right). \end{aligned}$$

When specialized to two first-variation solutions V and W at ϕ , $d\alpha_1(\phi)(V, W)$ vanishes, because for each interior point (i, j) all four rectangles touching it are contained in U , and

$V(\square^l) = V(i, j)$ and $W(\square^l) = W(i, j)$. Therefore, $d\alpha_1 = 0$ and the equation $d^2\mathcal{S} = 0$ becomes $d\alpha_2 = 0$, which in turn is equivalent to

$$\sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} [(j^2\phi)^*(j^2w \lrcorner j^2v \lrcorner \Omega_L^l)](\square^l) \right) = 0 \tag{4.12}$$

for all vector fields v, w on Y . This is the discrete analog of the multisymplectic form formula for the continuous space–time.

We observe that $dL = \Theta_L^1 + \Theta_L^2 + \Theta_L^3 + \Theta_L^4$, which shows that

$$\Omega_L^1 + \Omega_L^2 + \Omega_L^3 + \Omega_L^4 = 0,$$

which in turn implies that only three of the 2-forms $\Omega_L^l, l = 1, 2, 3, 4$, are in fact independent. In addition, this implies that for a *given and fixed* rectangle \square ,

$$\begin{aligned} 0 &= \sum_{l=1}^4 \pi_{\square}^* \Omega_L^l(\phi)(V, W) \\ &= \sum_{l=1}^4 \sum_{k=1}^4 \frac{\partial^2 L}{\partial y_k \partial y_l}(\phi(\square^1) \cdots \phi(\square^4))(V(\square^k)W(\square^l) - V(\square^l)W(\square^k)) \end{aligned}$$

for all sections ϕ and all vectors V, W .

4.6. Discrete Noether’s theorem

We would like to derive the discrete version of the Noether’s theorem for second-order field theories. This is not the most general form possible as we are working with a particular example. However, it is such as to facilitate the derivation of any other case without significant effort.

Suppose that a Lie group G with a Lie algebra \mathfrak{g} acts on Y by vertical symmetries such that the Lagrangian L is invariant under the action. Vertical action simply means that the base elements from X are not altered under the action, hence the action restricts to each fiber of Y . Let $\Phi : G \times Y \rightarrow Y$ denote the action of G on Y . For every $g \in G$, let $\Phi_g : Y \rightarrow Y$ be given by $y_{ij} \mapsto \Phi(g, y_{ij})$. We also use the notation $g \cdot y = \Phi_g(y)$ for the action. Then there is an induced action of G on \mathcal{B} defined in a natural way:

$$g \cdot (y_1, y_2, y_3, y_4) = (\Phi(g, y_1), \Phi(g, y_2), \Phi(g, y_3), \Phi(g, y_4)).$$

Recall that the infinitesimal generator of an action (of a Lie group G on a manifold M) corresponding to a Lie algebra element $\xi \in \mathfrak{g}$ is the vector field ξ_M on M obtained by differentiating the action with respect to g at the identity in the direction ξ . By the chain rule,

$$\xi_M(z) = \left. \frac{d}{dt} \right|_{t=0} [\exp(t\xi) \cdot z],$$

where \exp is the Lie algebra exponential map.

Using this formula, we immediately see that

$$\xi_{\mathcal{B}} \lrcorner dL = (\xi_Y(y_1), \xi_Y(y_2), \xi_Y(y_3), \xi_Y(y_4)).$$

The invariance of the Lagrangian under the action implies that

$$\xi_{\mathcal{B}} \lrcorner dL = 0 \quad \forall \xi \in \mathfrak{g},$$

which, for a given \square , is equivalent to

$$\sum_{l=1}^4 \frac{\partial L}{\partial y_l}(y_1, y_2, y_3, y_4) \xi_Y(y_l) = 0 \tag{4.13}$$

for all $\xi \in \mathfrak{g}$ and all $(y_1, y_2, y_3, y_4) \in \mathcal{B}$. For each l , let us denote by $\pi_{\square^l} : \mathcal{B} \rightarrow Y$ the projection onto the l th component. Using this projection the four components of the infinitesimal generator $\xi_{\mathcal{B}}$ are expressed as

$$\xi_{\mathcal{B}} = \sum_{l=1}^4 \xi_{\mathcal{B}}^l = \sum_{l=1}^4 (\xi_Y \circ \pi_{\square^l}) \frac{\partial}{\partial y_l}.$$

Hence, Eq. (4.13) becomes

$$\sum_{l=1}^4 \xi_{\mathcal{B}}^l \lrcorner \Theta_L^l = 0 \quad \forall \xi \in \mathfrak{g}. \tag{4.14}$$

We observe that for each l ,

$$\xi_{\mathcal{B}}^l \lrcorner \Theta_L^l = \frac{\partial L}{\partial y_l} \cdot (\xi_Y \circ \pi_{\square^l})$$

is a function on \mathcal{B} which we denote by $J^l(\xi)$. Notice that $J^l(\xi) = \xi_{\mathcal{B}}^l \lrcorner \Theta_L^l$ is the discrete multisymplectic analog of $\xi_M \lrcorner \omega_L = dJ(\xi)$ in classical mechanics so that ξ_M is the global Hamiltonian vector field of $J(\xi)$. Many symmetry groups act by special canonical transformations, i.e., $\mathfrak{L}_{\xi_M} \theta_L = 0$, in which case $J(\xi) = \xi_M \lrcorner \theta_L$. In a such case, $J(\xi)$ is uniquely defined.

Since $\xi_{\mathcal{B}}$ is linear in ξ , so are the functions $J^l(\xi)$, and we can replace the Lie group action by a Lie algebra action $\xi \mapsto \xi_{\mathcal{B}}$. Finally, we are ready to define the momentum maps.

Definition 4.4. There are four \mathfrak{g}^* -valued *momentum mappings* \mathbb{J}^l , $l = 1, 2, 3, 4$ on \mathcal{B} defined by

$$\langle \mathbb{J}^l(y_1, y_2, y_3, y_4), \xi \rangle = J^l(\xi)(y_1, y_2, y_3, y_4) \tag{4.15}$$

for all $\xi \in \mathfrak{g}$ and $(y_1, y_2, y_3, y_4) \in \mathcal{B}$, where $\langle \cdot, \cdot \rangle$ is the duality pairing.

Eq. (4.14) implies that

$$\mathbb{J}^1 + \mathbb{J}^2 + \mathbb{J}^3 + \mathbb{J}^4 = 0,$$

so, as in the case of the Lagrangian 2-forms, only three of the four momenta are essentially distinct.

The discrete version of the Noether theorem for second-order field theories now follows. Define the action of the Lie group G on \mathcal{C}_U by

$$g \cdot \phi \equiv \Phi_g \circ \phi, \text{ i.e. } (g \cdot \phi)(i, j) = \Phi(g, \phi(i, j)),$$

since the Lagrangian is G -invariant, so

$$\begin{aligned} \mathcal{S}(g \cdot \phi) &= \sum_{\square \subseteq U} L \circ j^2(g \cdot \phi)(\square^1) = \sum_{\square \subseteq U} L(g \cdot \phi(\square^1) \cdots g \cdot \phi(\square^4)) \\ &= \sum_{\square \subseteq U} L(\phi(\square^1) \cdots \phi(\square^4)) = \mathcal{S}(\phi). \end{aligned}$$

Once again letting $g = \exp(t\xi)$ and differentiating with respect to t at $t = 0$, we obtain that $(\xi_{\mathcal{C}_U} \lrcorner d\mathcal{S})(\phi) = 0 \ \forall \phi \in \mathcal{C}_U$. One can readily verify that $\xi_{\mathcal{C}_U}(\phi) = \xi_Y \circ \phi$, which is an element of $T_\phi \mathcal{C}_U$. Thus,

$$d\mathcal{S}(\phi) \cdot (\xi_Y \circ \phi) = 0 \tag{4.16}$$

for all $\xi \in \mathfrak{g}$ and $\phi \in \mathcal{C}_U$. Since \mathcal{S} is G -invariant, then G sends critical points of \mathcal{S} to themselves, or in other words, the action restricts to the space of solutions of the Euler–Lagrange equations. Therefore, if ϕ is a solution, so is $\phi^t \equiv \exp(t\xi) \cdot \phi$, where $\phi^0 = \phi$ and $(d/dt)|_{t=0} \phi^t = \xi_Y \circ \phi$. Substituting ϕ^t into the discrete Euler–Lagrange equations and differentiating with respect to t at $t = 0$, we obtain that for any ξ and ϕ , $\xi_Y \circ \phi$ is a first-variation equation solution. Using (4.8), (4.16) becomes

$$\begin{aligned} 0 = d\mathcal{S}(\phi) \cdot (\xi_Y \circ \phi) &= \sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} \frac{\partial L}{\partial y_l}(\phi(\square^1) \cdots \phi(\square^4)) \xi_Y \circ \phi(\square^l) \right) \\ &= \sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} (\xi_Y \lrcorner \Theta_L^l)(\phi(\square^1) \cdots \phi(\square^4)) \right) \\ &= \sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} \mathbb{J}^l(\phi(\square^1) \cdots \phi(\square^4))(\xi) \right) \end{aligned}$$

for all ϕ from the solution space and all ξ . Thus, the discrete version of the Noether’s theorem is

$$\sum_{(i,j) \in \partial U} \left(\sum_{\square \subseteq U; l; (i,j) = \square^l} [(j^2\phi)^* \mathbb{J}^l](\square^1) \right) = 0 \tag{4.7}$$

for all ϕ from the solution space.

Acknowledgements

The authors would like to thank the Center for Nonlinear Studies at Los Alamos, where most of this work was completed, for providing a wonderful working environment. SS was partially supported by NSF-KDI grant ATM-98-73133 and the DOE.

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