Generating Functionals and Lagrangian PDEs

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Dedicated to the memory of Jerrold E. Marsden.

Abstract

We introduce the concept of Type-I/II generating functionals defined on the space of boundary data of a Lagrangian field theory. On the Lagrangian side, we define an analogue of Jacobi's solution to the Hamilton-Jacobi equation for field theories, and we show that by taking variational derivatives of this functional, we obtain an isotropic submanifold of the space of Cauchy data, described by the so-called multisymplectic form formula. We also define a Hamiltonian analogue of Jacobi's solution, and we show that this functional is a Type-II generating functional. We finish the paper by defining a similar framework of generating functions for discrete field theories, and we show that for the linear wave equation, we recover the multisymplectic conservation law of Bridges.

1 Introduction

The aim of the paper is to establish a theory of "generating functionals" for classical Lagrangian field theories, playing a similar role to the generating functions in mechanics. Generating functions play an important role in mechanics, as a means of characterizing canonical transformations that preserve the structure of Hamilton's equations. A particularly important generating function is the one associated with the time-dependent symplectic map that trivializes the dynamics of a Hamiltonian system, which is described by

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the Hamilton–Jacobi equation. In turn, Jacobi's solution of the Hamilton–Jacobi equation can be viewed as a Type-I generating function which is given by the value of the action integral for paths that satisfy the boundary conditions and extremize the action. We will introduce a boundary Lagrangian for field theories that plays the role of Jacobi's solution, and demonstrate that functional derivatives of the boundary Lagrangian lead to expressions on the boundary of a space-time region that are analogous to the implicit expressions for a symplectic map expressed in terms of classical generating functions.

This has important implications for discrete mechanics, since Jacobi's solution to the Hamilton–Jacobi equation is the exact discrete Lagrangian [18], and the order of approximation of a variational integrator can be characterized by the extent to which a computable discrete Lagrangian approximates the exact discrete Lagrangian. As such, a precise characterization of the boundary Lagrangian is essential for the construction and analysis of variational integrators for Lagrangian field theories.

Geometry of the Space of Boundary Data To derive the expression for the boundary Lagrangian, we rely on the framework of Lawruk, Śniatycki and Tulczyjew [14], who describe the space of boundary data associated to a given PDE, showing among other things that a PDE determines an isotropic or sometimes even a Lagrangian submanifold of the space of all boundary data. Kijowski and Tulczyjew [12] connect these results with the polysymplectic description of field theories and give a description in terms of generating functionals similar to the ones defined in this paper. In this formalism, a fixed Riemannian connection is needed to introduce the Hamiltonian formulation, but the introduction of metrics, connections, or other background objects might not be desirable when the goal is to describe a generally covariant theory (i.e., a theory which is invariant under arbitrary diffeomorphisms of spacetime; see [17] for a discussion of general covariance in field theories). One of the aims of this paper, therefore, is to recast these results in the multisymplectic formalism, where no extraneous background objects are needed for the Hamiltonian description.

In recent years, Rovelli [22] has rediscovered many of these results in his search for a Hamiltonian description of field theories in which no space-time split is made. He applied this formalism to general relativity using Ashtekar variables, rederiving among other things the Einstein-Hamilton-Jacobi equation. Our approach agrees with Rovelli's results wherever appropriate, but one of the advantages of the multisymplectic approach used here is that we are easily able to tie in our results with infinite-dimensional symplectic geometry.

Inspired by these papers we introduce in this paper Type-I and Type-II generating functionals. While the technical details are given below, the idea is that for any given Lagrangian PDE we can define a functional $L_{\partial U}$, and by taking the exterior derivative, a one-form

$$\mathbf{d}L_{\partial U} : \mathcal{Y}_{\partial U} \to T^*\mathcal{Y}_{\partial U} \tag{1.1}$$

which takes Dirichlet boundary on ∂U (the elements of $\mathcal{Y}_{\partial U}$) into the corresponding Neumann data along ∂U (the elements of $T^*\mathcal{Y}_{\partial U}$). We call the functional $L_{\partial U}$ appearing in (1.1) a Type-I generating functional. The image of this map turns out to be an isotropic submanifold of $T^*\mathcal{Y}_{\partial U}$ (and in some cases even a Lagrangian submanifold), so that the pull-back along $\mathbf{d}L_{\partial U}$ of the canonical symplectic form ω on $T^*\mathcal{Y}_{\partial U}$ vanishes:

$$(\mathbf{d}L_{\partial U})^*\omega = 0 \tag{1.2}$$

If instead we prescribe mixed boundary conditions along ∂U, we refer to the corresponding functional as a Type-II generating functional. Taking variational derivatives of this functional will then yield the Dirichlet boundary conditions along the part of ∂U where Neumann boundary conditions have been specified, and vice versa. The resulting map again determines an isotropic submanifold of $T^*\mathcal{Y}_{\partial U}$, so that a result similar to (1.2) holds.

Generating Functionals and Multisymplecticity. The second goal of this paper is to shed further light on the *multisymplectic form formula.* This formula was introduced in [19] as a criterion for when the space of solutions of a PDE conserves a given multisymplectic form. Concretely, in the case of field theories derived from a Lagrangian function L, the multisymplectic form formula takes on the following form. If Ω_L is the *Lagrangian multisymplectic form* (defined below in (1.5) and (1.6)), then for any subset U of the space of independent variables, and for any solution ϕ of the Euler-Lagrange equations defined on U, we have that

$$\int_{\partial U} (j^1\phi)^* \left(\mathbf{i}_{j^1W}\mathbf{i}_{j^1V}\Omega_L\right) = 0, \tag{1.3}$$

where V and W are arbitrary first variations of ϕ. If we restrict to vertical first variations, this formula takes on the following form in coordinates:

$$\int_{\partial U} \frac{\partial^2 L}{\partial y^a_\mu \partial y^b_\nu}(V^a(x)W^b_{,\nu}(x) - W^a(x)V^b_{,\nu}(x))d^nx_\mu = 0,$$

where V^a, W^b are the components of V and W, and the subscript ν denotes differentiation with respect to x^ν.

For Hamiltonian field theories on the other hand, Bridges [3] defined a different notion of multisymplecticity. In this context, a set of Hamiltonian PDEs is said to be multisymplectic if they satisfy a certain differential conservation law. Under some restrictions, this conservation law can be rewritten in integral form to yield a result similar to (1.3), but the precise link between both formulations in full generality is not yet clear.

In this paper we take a different approach to the derivation of (1.3) and its implications. Given a Lagrangian field theory, we construct the associated generating functional (1.1) and we relate this functional to the integral of the Poincaré-Cartan form Θ_L over the boundary ∂U. In this way, we then show that the left-hand side of the isotropy condition (1.2), when written out in terms of the multisymplectic form $\Omega_L = -\mathbf{d}\Theta_L$, is nothing but the multisymplectic form formula (1.3).

The advantage of this approach is that it provides a criterion of multisymplecticity which can be applied to any set of PDEs for which a Dirichlet-to-Neumann map can be defined. From our point of view, therefore, the isotropy condition (1.2) is fundamental, and the multisymplectic form formula (1.3) arises as a consequence.

Outlook: Discrete Lagrangian Field Theories. Our long-term goal is to clarify the concept of multisymplecticity for discrete Lagrangian field theories, in which the space of independent variables is replaced by a discrete mesh. While both the criterion of Bridges (see [4, 5] and the references therein) as well as the multisymplectic form formula[1] can be defined in this context, the relation between both is not clear yet. In the discrete context, we show that a generating functional akin to the one described in (1.1) can be introduced and that its image determines an isotropic submanifold of the space of (finite-dimensional) discrete boundary data. As in the case of continuous field theories, the condition of isotropy then gives rise to the discrete multisymplectic form formula. While we have not yet been able to establish the link between this condition and Bridges' discrete version of multisymplecticity in full generality, we finish the paper with a simple discretization of the wave equation where this link can be established by direct computation.

Dedication. We dedicate this paper to the memory of Jerrold E. Marsden. The methods pioneered by Jerry and his collaborators exerted a very profound influence on this paper: for the treatment of the infinite-dimensional geometry of the space of boundary data, we relied heavily on the foundational results from [1, 7], while the connection with field theory, and in particular the variational/multisymplectic formulation, uses the results from the GIMMSY manuscripts [10, 11]. In more recent years, Jerry was influential in the development of variational principles for discrete field theories, his paper [19] being the first to give a definition of multisymplecticity for a discrete Lagrangian field theory.

The Geometry of Lagrangian Field Theories

In this section, we briefly recall the fiber bundle approach to classical field theory. We give a description in local coordinates; for a intrinsic description, as well as applications and a more in-depth discussion, see [2, 6, 10, 11] and the references therein.

Throughout this paper, we will consider fields as sections of a fiber bundle $\rho : Y \to X$. Often, X will be spacetime and Y will be the product of X with a vector space V, but this

[1]It is interesting to note from a historical point of view that a precursor of the multisymplectic form formula already appears in the seminal work of Courant, Friedrichs and Lewy [8].

will not always be the case. We write the dimension of X as $n+1$, with $n \geq 0$, and we denote coordinates on X by (x^μ), $\mu = 0, \ldots, n$. We use the shorthand $d^{n+1}x = dx^0 \wedge \cdots \wedge dx^n$, and we put

$$\begin{aligned} d^n x_\mu &:= \mathbf{i}_{\partial/\partial x^\mu} d^{n+1}x \\ &= (-1)^\mu dx^0 \wedge \cdots \wedge dx^{\mu-1} \wedge dx^{\mu+1} \wedge \cdots \wedge dx^n, \end{aligned} \tag{1.4}$$

so that (up to sign) $d^n x_\mu$ is $d^{n+1}x$ with the dx^μ term removed.

On Y we choose coordinates (x^μ, y^a), $a = 1, \ldots, k$, adapted to the projection ρ, so that a section $\phi : X \to Y$ can be locally written as $\phi(x) = (x^\mu, \phi^a(x))$, with $\phi^a(x)$ locally defined component functions.

We define the first jet bundle J^1Y to consist of equivalence classes of local sections of π, where two sections $\phi, \phi' : X \to Y$ are equivalent at a point $x \in X$ if their first-order Taylor expansions around x agree, i.e., $T_x\phi = T_x\phi'$. On J^1Y, we have local coordinates (x^μ, y^a, y^a_μ), where the y^a_μ can be considered as the derivatives of y^a with respect to the variables x^μ, which we refer to as multi-velocities. Given a local section $\phi : X \to Y$ of ρ, we define the prolongation of ϕ to be the section $j^1\phi$ of J^1Y given in local coordinates by

$$j^1\phi(x) = \left(x^\mu, \phi^a(x), \frac{\partial \phi^a}{\partial x^\mu}(x) \right),$$

where the $\phi^a(x)$ are the component functions of ϕ.

By a Lagrangian density on J^1Y we mean a map $\mathcal{L} : J^1Y \to \bigwedge^{n+1}(X)$, where $\bigwedge^{n+1}(X)$ is the space of volume forms on X. Such a Lagrangian density can be written in local coordinates as $\mathcal{L}(x^\mu, y^a, y^a_\mu) = L(x^\mu, y^a, y^a_\mu)\, d^{n+1}x$, where $L(x^\mu, y^a, y^a_\mu)$ is a function on J^1Y referred to as the Lagrangian function.

Given a Lagrangian density $\mathcal{L}$, we can introduce a number of geometric objects on the first jet bundle. In local coordinates, the Poincaré-Cartan form is given by

$$\Theta_L = \left(L - \frac{\partial L}{\partial y^a_\mu} y^a_\mu \right) d^{n+1}x + \frac{\partial L}{\partial y^a_\mu} dy^a \wedge d^n x_\mu. \tag{1.5}$$

We define the multisymplectic form Ω_L on J^1Y by

$$\Omega_L = -\mathbf{d}\Theta_L. \tag{1.6}$$

The expression (1.5) for the Poincaré-Cartan form can be rewritten as

$$\Theta_L = L d^{n+1}x + \frac{\partial L}{\partial y^a_\mu}(dy^a - y^a_\nu dx^\nu) \wedge d^n x_\mu, \tag{1.7}$$

since from (1.4) it follows that $dx^\nu \wedge d^n x_\mu = \delta^\nu_\mu d^{n+1}x$, with δ^ν_μ the Kronecker delta. The advantage of this expression is that the forms $dy^a - y^a_\nu dx^\nu$ which appear in the second term are *contact forms*, i.e., they vanish when pulled back along a prolongated section: if $j^1\phi(x) = (x, \phi^a(x), \partial\phi^a(x)/\partial x^\mu)$ in local coordinates, then

$$(j^1\phi)^*(dy^a - y^a_\nu dx^\nu) = d\phi^a(x) - \frac{\partial\phi^a(x)}{\partial x^\nu}dx^\nu = 0.$$

Along prolongated sections, we therefore have that

$$(j^1\phi)^*\Theta_L = (j^1\phi)^*(Ld^{n+1}x). \tag{1.8}$$

This equality will often be useful later on.

2 The Space of Boundary Data

Let U be an open subset of X with boundary ∂U. We want to prescribe boundary data along ∂U with values in Y, the total space of the configuration bundle $\rho : Y \to X$. We first describe the geometry of the space of all boundary data, and then we discuss some related spaces. We emphasize that at this stage, ∂U does not have to be a Cauchy surface, or even be spacelike: indeed, all of the definitions below are independent of the choice of a metric on X, so that in particular they can be applied to hyperbolic and elliptic problems alike.

By an ***element of boundary data*** on U, we mean a section $\varphi : \partial U \to Y$ of ρ, defined on the boundary of U. We denote by $\mathcal{Y}_{\partial U}$ the space of all boundary data and we now describe the tangent and cotangent bundles of this space. We can describe the tangent vectors $\delta\varphi$ at a point $\varphi \in \mathcal{Y}_{\partial U}$ as follows: let φ_ϵ be a curve in $\mathcal{Y}_{\partial U}$ such that $\varphi_{\epsilon=0} = \varphi$, and put

$$\delta\varphi(x) := \frac{d\varphi_\epsilon(x)}{d\epsilon}\Big|_{\epsilon=0}$$

for all $x \in \partial U$. Note that the right-hand side takes values in the space of vertical tangent vectors: as each map φ_ϵ is a section of ρ, we have that $\rho \circ \varphi_\epsilon = \mathrm{Id}$, and therefore

$$T\rho(\delta\varphi(x)) = \frac{d}{d\epsilon}\Big|_{\epsilon=0}\rho(\varphi_\epsilon(x)) = 0.$$

As the right-hand side takes values in $V_{\varphi(x)}Y$, we have that $\delta\varphi$ is a map from ∂U into VY with the property that $\delta\varphi(x) \in V_{\varphi(x)}Y$ for all $x \in \partial U$. These maps can alternatively be described as vector fields along φ, or as sections of the pullback bundle $\varphi^*(VY)$. In any case, we have that the tangent space at a point is given by

$$T_\varphi\mathcal{Y}_{\partial U} = \left\{\delta\varphi : \partial U \to VY : \delta\varphi(x) \in V_{\varphi(x)}Y \quad \text{for all } x \in \partial U\right\}.$$

In local coordinates, an element $\delta\varphi$ of $T_\varphi \mathcal{Y}_{\partial U}$ is given by

$$\delta\varphi(x) = \delta\varphi^a(x) \frac{\partial}{\partial y^a},$$

where the $\delta\varphi^a(x)$ are locally defined component functions. Roughly speaking, we can think of the elements $\delta\varphi \in T_\varphi \mathcal{Y}_{\partial U}$ as *infinitesimal variations* of the boundary data given by φ. Following [2], we will refer to $T\mathcal{Y}_{\partial U}$ as the space of ***Cauchy data***.

We now describe the dual spaces $T^*_\varphi \mathcal{Y}_{\partial U}$. We restrict ourselves to the smooth dual, in other words, the space of smooth linear functionals from $T_\varphi \mathcal{Y}_{\partial U}$ to $\mathbb{R}$. Since the elements of $T_\varphi \mathcal{Y}_{\partial U}$ are vertical vector fields along ∂U, the elements of the dual can be identified with linear maps π from the space of vertical vector fields to the space of densities on the boundary, so that the duality pairing can be defined in terms of integration over the boundary by

$$\langle \delta\varphi, \pi \rangle = \int_{\partial U} \pi \cdot \delta\varphi. \tag{2.1}$$

Here, $\pi \cdot \delta\varphi$ is the volume form on ∂U obtained by letting the linear map π act on the vertical vector field $\delta\varphi$.

We now make this picture more precise. To describe $T^*_\varphi \mathcal{Y}_{\partial U}$, we consider first the tensor product bundle $\varphi^*(V^*Y) \otimes \bigwedge^n(\partial U)$, where V^*Y is the dual bundle to the vertical bundle VY, $\varphi^*(V^*Y)$ is the pullback bundle over ∂U, and $\bigwedge^n(\partial U)$ is the bundle of volume forms (densities) on the boundary ∂U, viewed as a bundle over Y. Note that if there is a locally defined volume form dS on ∂U, then the elements of $\varphi^*(V^*Y) \otimes \bigwedge^n(\partial U)$ can be written locally as $\pi = \pi_a dy^a \otimes dS$.

We now let $T^*_\varphi \mathcal{Y}_{\partial U}$ be the space of sections of $V^*Y \otimes \bigwedge^n(\partial U)$, defined on the boundary ∂U. Each section $\pi \in T^*_\varphi \mathcal{Y}_{\partial U}$ is a map from ∂U into $\varphi^*(V^*Y) \otimes \bigwedge^n(\partial U)$, with the property that

$$\pi(x) \in V^*_{\varphi(x)} Y \otimes {\textstyle\bigwedge}^n_x(\partial U)$$

for all $x \in \partial U$. Again under the assumption that dS is a local volume form on ∂U, we have that π can be written locally as

$$\pi(x) = \pi_a dy^a \otimes dS. \tag{2.2}$$

For reasons that will become clear later on, we will refer to π as the momentum in the direction normal to ∂U, and we will refer to the cotangent bundle $T^*\mathcal{Y}_{\partial U}$ as the space of ***normal momenta***.

The duality pairing (2.1) between $T\mathcal{Y}_{\partial U}$ and $T^*\mathcal{Y}_{\partial U}$ can then be written as

$$\langle \delta\varphi, \pi \rangle = \int_{\partial U} \pi \cdot \delta\varphi = \int_{\partial U} \pi_a(x) \delta\varphi^a(x)\, dS.$$

For future reference, we point out that $T^*\mathcal{Y}_{\partial U}$ is equipped with a canonical weak symplectic form, given by $\omega = -\mathbf{d}\Theta$, where Θ is the one-form defined intrinsically as

$$\Theta(\pi)(\delta\pi) = \langle T\tau(\delta\pi), \pi \rangle\,, \tag{2.3}$$

for all $\pi \in T^*\mathcal{Y}_{\partial U}$ and $\delta\pi \in T_\pi(T^*\mathcal{Y}_{\partial U})$, where $\tau : T^*\mathcal{Y}_{\partial U} \to \mathcal{Y}_{\partial U}$ is the cotangent bundle projection (see [1]). Instead of this definition, we will often use the following defining property of Θ: for every one-form β on $\mathcal{Y}_{\partial U}$, we have that

$$\beta^*\Theta = \beta, \tag{2.4}$$

where on the left-hand side β is interpreted as a map from $\mathcal{Y}_{\partial U}$ into $T^*\mathcal{Y}_{\partial U}$.

3 The Boundary Lagrangian

Let $\mathcal{L} : J^1Y \to \bigwedge^{n+1}(X)$ be a first-order Lagrangian density and denote, as before, $\mathcal{L}(j^1\phi) = L(j^1\phi)\,dV$, with $L(j^1\phi)$ a scalar function on J^1Y. To make the distinction between boundary data on ∂U and fields defined on the interior of U, we will denote the former by $\varphi \in \mathcal{Y}_{\partial U}$, while the latter are denoted by ϕ.

We now define the ***boundary Lagrangian*** $L_{\partial U}$ as the functional on $\mathcal{Y}_{\partial U}$ given by

$$L_{\partial U}(\varphi) = \int_U L(j^1\phi)dV, \tag{3.1}$$

where ϕ is the unique section satisfying the Euler-Lagrange equations, and such that ϕ agrees with φ on ∂U:

$$\frac{d}{dx^\mu}\left(\frac{\partial L}{\partial y^a_\mu}(j^1\phi)\right) - \frac{\partial L}{\partial y^a}(j^1\phi) = 0 \quad \text{and} \quad \phi_{|\partial U} = \varphi. \tag{3.2}$$

In other words,

$$L_{\partial U}(\varphi) = \mathcal{S}(\phi), \tag{3.3}$$

where $\mathcal{S}$ is the action functional, and φ and ϕ are related as described in (3.2). This leads us to an alternative description of the boundary Lagrangian, which will often be useful in computations: as the solutions ϕ of the Euler-Lagrange equations are precisely the extremal points of the action functional $\mathcal{S}$, we see that $L_{\partial U}(\varphi)$ is precisely the extremal value of $\mathcal{S}$:

$$L_{\partial U}(\varphi) = \operatorname*{ext}_{\phi_{|\partial U} = \varphi} \mathcal{S}(\phi), \tag{3.4}$$

where the extremal value of $\mathcal{S}$ is computed over the class of all sections ϕ such that $\phi_{|\partial U} = \varphi$. Indeed, the variational characterization of the boundary Lagrangian is more broadly applicable than the characterization in terms of the action of the section that satisfies the boundary conditions and the Euler–Lagrange equations since in the case of degenerate Lagrangians, the section satisfying the boundary-value problem may not be unique, but the variational characterization remains well-defined.

The Space of Admissible Boundary Data. It will often happen that one cannot prescribe arbitrary boundary data for the Euler-Lagrange equations (3.2). We will denote by $\mathcal{K}_{\partial U}$ the space of boundary data that give rise to a unique solution of the Euler-Lagrange equations, and we refer to $\mathcal{K}_{\partial U} \subset \mathcal{Y}_{\partial U}$ as the space of ***admissible boundary data***. The specification of $\mathcal{K}_{\partial U}$ will depend on the type of PDE under study and the geometry of U. We give some examples at the end of this section.

Functional Derivatives. We define the functional derivative of $L_{\partial U}$ as follows: $\delta L_{\partial U}/\delta\varphi$ is the unique element of $T^*\mathcal{Y}_{\partial U}$ such that

$$\mathbf{d}L_{\partial U}(\varphi)\cdot\delta\varphi = \int_{\partial U} \frac{\delta L_{\partial U}}{\delta \varphi}\cdot\delta\varphi$$

for every variation $\delta\varphi \in T\mathcal{Y}_{\partial U}$, where $\mathbf{d}L_{\partial U}$ is the exterior derivative of the boundary Lagrangian. If not all boundary data are admissible, so that $\mathcal{K}_{\partial U}$ is a proper subset of $\mathcal{Y}_{\partial U}$, then the admissible variations $\delta\varphi$ are elements of $T\mathcal{K}_{\partial U}$, so that $\mathbf{d}L_{\partial U}(\varphi) \in T^*_\varphi\mathcal{K}_{\partial U}$.

By applying the exterior differential to both sides of (3.3), we now obtain

$$\mathbf{d}L_{\partial U}(\varphi)\cdot\delta\varphi = \mathbf{d}\mathcal{S}(\phi)\cdot\delta\phi,$$

where ϕ is the solution of the Euler-Lagrange equations with boundary data φ, and $\delta\phi$ is a ***first variation*** of ϕ, defined as follows. Let φ_ϵ be a curve in the space $\mathcal{Y}_{\partial U}$ of boundary data such that $\varphi_{\epsilon=0} = \varphi$ and $\frac{d}{d\epsilon}\varphi_\epsilon\big|_{\epsilon=0} = \delta\varphi$, and let ϕ_ϵ be the corresponding family of solutions of the Euler-Lagrange equations such that $(\phi_\epsilon)_{|\partial U} = \varphi_\epsilon$. Then $\delta\phi$ is given by

$$\delta\phi(x) = \frac{d\phi_\epsilon(x)}{d\epsilon}\bigg|_{\epsilon=0}, \tag{3.5}$$

for all $x \in \partial U$. Explicitly, the first variations $\delta\phi$ satisfy the first-variation equation, obtained by linearizing the Euler-Lagrange equations.

The exterior differential of the action functional is given by the first variation formula:

$$\begin{aligned}\mathbf{d}\mathcal{S}(\phi)\cdot\delta\phi &= \int_U \left(\frac{\partial L}{\partial y^a}\delta y^a + \frac{\partial L}{\partial y^a_\mu}\delta y^a_\mu\right)\, d^{n+1}x \\ &= \int_U \left(\frac{\partial L}{\partial y^a} - \frac{d}{dx^\mu}\left(\frac{\partial L}{\partial y^a_\mu}\right)\right)\delta y^a\, d^{n+1}x + \int_{\partial U}\frac{\partial L}{\partial y^a_\mu}\delta y^a\, d^n x_\mu.\end{aligned}$$

As ϕ is a solution of the Euler-Lagrange equations, the integral over U vanishes and we conclude that

$$\mathbf{d}L_{\partial U}(\varphi)\cdot\delta\varphi = \int_{\partial U}\frac{\partial L}{\partial y^a_\mu}\delta y^a\, d^n x_\mu, \tag{3.6}$$

and therefore

$$\frac{\delta L_{\partial U}}{\delta \varphi} = \frac{\partial L}{\partial y^a_\mu} dy^a \otimes \iota^* \left(d^n x_\mu \right), \tag{3.7}$$

where $\iota : \partial U \hookrightarrow X$ is the embedding of the boundary ∂U into X. Since $d^n x_\mu$ is an n-form on X, its pullback along ι is a form of maximal degree on ∂U. If we choose coordinates on X that are adapted to ∂U, in the sense that ∂U is locally given by $x^0 = 0$, then ι is locally given by $\iota(x^1, \ldots, x^n) = (0, x^1, \ldots, x^n)$, so that

$$\iota^* \left(d^n x_0 \right) = d^n x_0, \quad \text{and} \quad \iota^* \left(d^n x_i \right) = 0 \quad (i = 1, \ldots, n).$$

As a result, in adapted coordinates we have that

$$\frac{\delta L_{\partial U}}{\delta \varphi} = \frac{\partial L}{\partial y^a_0} dy^a \otimes d^n x_0.$$

A more intrinsic expression may be given when X is equipped with a metric tensor, as we now show.

Normal Momenta. When a Riemannian or Lorentzian metric G on X is given, we may describe the functional derivatives as follows. In both cases, we have that

$$\iota^*(d^n x_\mu) = n_\mu \, dS,$$

(see [23]), where n^μ is the outward normal to ∂U, dS is the induced metric volume form on ∂U, and indices are raised/lowered using the metric. The functional derivatives (3.7) can then be written as

$$\pi := \frac{\delta L_{\partial U}}{\delta \varphi} = \frac{\partial L}{\partial y^a_\mu} n_\mu \, dy^a \otimes dS,$$

so that by comparing with (2.2), we have for the components

$$\pi_a = \frac{\partial L}{\partial y^a_\mu} n_\mu = p^\mu_a n_\mu.$$

In other words, the boundary momentum π_a is the normal component of the spacetime momentum p^μ_a, so that we will refer to $\pi \in T^* \mathcal{Y}_{\partial U}$ as the ***normal momentum*** to the boundary ∂U.

Multisymplectic Form Formula. A more careful derivation of (3.6) proceeds as follows. The boundary Lagragian $L_{\partial U}$ can be written in terms of the Poincaré-Cartan form Θ_L as

$$L_{\partial U}(\varphi) = \int_{\partial U} (j^1 \phi)^* \Theta_L$$

where ϕ is the solution of the Euler-Lagrange equations with boundary data φ, and $j^1\phi$ is its first jet prolongation. Here, we have used (1.8) to bring in the Poincaré-Cartan form.

By taking the exterior derivative, we then obtain

$$\mathbf{d}L_{\partial U}(\varphi) \cdot \delta\varphi = \int_{\partial U} (j^1\phi)^* \left(\mathbf{i}_{j^1 V}\Theta_L\right), \tag{3.8}$$

where the vector field V is a first variation of the solution ϕ, defined as before in (3.5). The advantage of this expression is that we can now take the exterior derivative again, to obtain

$$\mathbf{d}^2 L_{\partial U}(\varphi) \cdot (\delta\varphi, \delta\varphi') = \int_{\partial U} (j^1\phi)^* \left(\mathbf{i}_{j^1 W}\mathbf{i}_{j^1 V}\Omega_L\right), \tag{3.9}$$

where V and W are the first variations induced by $\delta\varphi$ and $\delta\varphi'$, respectively. The proof of this results proceeds along similar lines as the proof of Lemma 5.1 in [11]. Since $\mathbf{d}^2 \equiv 0$, we now have that

$$\int_{\partial U} (j^1\phi)^* \left(\mathbf{i}_{j^1 W}\mathbf{i}_{j^1 V}\Omega_L\right) = 0, \tag{3.10}$$

for all solutions ϕ of the Euler-Lagrange equations, and all first variations V, W. This is the ***multisymplectic form formula***, first proposed in [19]. Our derivation is close in spirit to the one in that paper, because of the link between the boundary Lagrangian and the action functional. In Section 4 we will see the multisymplectic form formula appear under a different guise, as the condition for the manifold of physical solutions to be an isotropic submanifold of the space of normal momenta.

We finish by noting that our version of the multisymplectic form formula is somewhat less general than the one derived in [19], since we consider only vertical variations. However, as one of the motivations for this work is the derivation of a multisymplectic form formula for discrete field theories, for which infinitesimal horizontal variations are not really well-defined, this is not a fundamental restriction.

Relation with the Crnković-Witten Symplectic Form. As pointed out by Rovelli [22], the Crnković-Witten symplectic form on the solution space can be related to the various structures on the space of boundary data. We present here a slightly different approach from Rovelli, emphasizing the link with the multisymplectic form formula.

We assume that the base space X is equipped with a Lorentzian metric and we let U be a region bounded by two spacelike hypersurfaces, Σ_+ and Σ_-. We choose the orientation so that $\partial U = \Sigma_+ - \Sigma_-$, and we consider a boundary Lagrangian $L_{\partial U}$ for this particular geometry. In Wheeler's terminology [20], U would be called a "thick sandwich."

From the expression (4.1), to be proved below, for the pullback $(\mathbf{d}L_{\partial U})^*\omega$, or alternatively from the multisymplectic form formula (3.10) directly, we have that

$$\int_{\Sigma_-} (j^1\phi)^* \left(\mathbf{i}_{j^1 W}\mathbf{i}_{j^1 V}\Omega_L\right) = \int_{\Sigma_+} (j^1\phi)^* \left(\mathbf{i}_{j^1 W}\mathbf{i}_{j^1 V}\Omega_L\right),$$

for all solutions ϕ of the Euler-Lagrange equations, and first variations V, W. These expressions, however, are nothing but the symplectic structures of Crnkovic-Witten [9] and Zuckerman [24] on the space of solutions associated to L, integrated respectively over Σ_- and Σ_+. We have therefore shown that the definition of this symplectic structure is independent of the spatial hypersurface along which to integrate. This conclusion is of course not new, but the link with the multisymplectic form formula has hitherto not been established.

Examples

For most field theories, the boundary Lagrangian (3.1) cannot be computed explicitly. Here we present a number of examples where this is possible after all.

Mechanics. In the case of a mechanical system on a configuration space Q and with regular Lagrangian $L(q, v) : TQ \to \mathbb{R}$, we let X be $\mathbb{R}$ and we take for Y the product $\mathbb{R} \times Q$. The projection $\rho : Y \to X$ is then the projection onto the first factor.

We let U be an open subset of $X = \mathbb{R}$ and we assume without loss of generality that U is an interval $(0, h)$, so that $\partial U = \{0, h\}$. In this case, the space of boundary data is just the product $Q \times Q$, where we think of the first, resp. the second factor, as specifying the configuration of the system at $t = 0, h$, respectively. Accordingly, the space of normal momenta is given by $T^*Q \times T^*Q$. If L is nondegenerate and h is small enough, then it is well known that for every pair (q_0, q_1) in $Q \times Q$ there exists a unique solution $q(t)$ of the Euler-Lagrange equations so that $q(0) = q_0$ and $q(h) = q_1$ (see, for instance, [18]).

According to the definition (3.1), the boundary Lagrangian is then given by

$$L_{\partial U}(q_0, q_1) := \int_0^h L(q(t), \dot{q}(t))dt,$$

where $q(t)$ is the unique solution of the Euler-Lagrange equations with boundary data (q_0, q_1). In this way, we recover the *exact discrete Lagrangian* introduced in [18]. The variational derivatives (3.7) are

$$\frac{\delta L_{\partial U}}{\delta q_0} = -\frac{\partial L}{\partial \dot{q}}(q(0), \dot{q}(0)), \quad \text{and} \quad \frac{\delta L_{\partial U}}{\delta q_1} = \frac{\partial L}{\partial \dot{q}}(q(h), \dot{q}(h)),$$

and coincide with the momenta of the system at the begin and end point of the solution trajectory $q(t)$, $t \in [0, h]$. The minus sign is due to the orientation of the boundary $\{0, h\}$. Notice that these equations are precisely the implicit characterization of a symplectic map, where $L_{\partial U}$ is viewed as a Type-I generating function.

Harmonic Functions. Consider secondly the case of harmonic functions on $\mathbb{R}^n$, for which the Lagrangian is given by

$$L(\phi, \nabla\phi) = \frac{1}{2} \|\nabla\phi\|^2$$

so that the field equations are given by Laplace's equation, $\Delta\phi = 0$. The action is then given by

$$\mathcal{S}(\phi) = \frac{1}{2}\int_U \|\nabla\phi\|^2 \, dV = \frac{1}{2}\int_{\partial U} \phi\frac{\partial\phi}{\partial n}\, dl - \frac{1}{2}\int_U \phi\Delta\phi\, dV,$$

where we have used the divergence theorem, with $\partial\phi/\partial n := n\cdot\nabla\phi$ the normal derivative. If we let ϕ be a solution of Laplace's equation with prescribed boundary data φ on ∂U, we obtain for the boundary Lagrangian (3.1)

$$L_{\partial U}(\varphi) = \frac{1}{2}\int_{\partial U} \varphi\frac{\partial\phi}{\partial n}\, dl, \tag{3.11}$$

so that the variational derivative becomes

$$\frac{\delta L_{\partial U}}{\delta\varphi} = \frac{\partial\phi}{\partial n}\, d\phi\otimes dl,$$

where dl is the Euclidian line element along ∂U. We conclude that the map which associates to each element of boundary data φ the corresponding variational derivative $\delta L_{\partial U}/\delta\varphi$ is nothing but the *Dirichlet-to-Neumann map* of the Laplace equation. Last, if $n \geq 3$, the boundary Lagrangian (3.1) can also be formally related to the *harmonic capacity* of the domain U.

The Wave Equation. Our last example concerns the wave equation $\phi_{tt} - \phi_{xx} = 0$, with Lagrangian

$$L(\phi, \phi_{,\mu}) = \frac{1}{2}(\phi_{,t}^2 - \phi_{,x}^2). \tag{3.12}$$

Our exposition follows [12, 14]. We assume that U is a square in $\mathbb{R}^2$ of unit length whose corner vertices are given by $(0,0), (1,0), (1,1), (0,1)$ and we prescribe boundary data $\varphi(t,x)$ along ∂U. An arbitrary solution to the linear wave equation can be written as $\phi(t,x) = F(x-t) + G(x+t)$, where F and G are determined through the boundary conditions by

$$F(x) + G(x) = \varphi(0,x), \quad F(x-1) + G(x+1) = \varphi(1,x),$$

and

$$F(-t) + G(t) = \varphi(t,0), \quad F(1-t) + G(1+t) = \varphi(t,1).$$

Note that for F and G to be determined from this set of equations, the boundary data needs to satisfy the following compatibility condition:

$$\varphi(t,0) + \varphi(1-t,1) - \varphi(0,x) - \varphi(1,1-x) = 0. \tag{3.13}$$

For the unit square U, the space of admissible boundary data $\mathcal{K}_{\partial U}$ is therefore the space of all smooth functions on the boundary ∂U that satisfy this condition. By substituting the solution of the wave equation with given boundary data φ back into the action density (3.12), we then obtain the following expression for the boundary Lagrangian:

$$L_{\partial U}(\varphi) = \int_0^1 \big(\varphi_x(\alpha, 0) - \varphi_t(0, \alpha)\big)\big(\varphi(1-\alpha, 1) - \varphi(0, \alpha)\big)\, d\alpha.$$

If the boundary of U consists (partly) of characteristic curves of the wave equation, then the wave equation will still be well-posed, but more restrictive compatibility conditions will arise. Assume, for instance, that U is the diamond shape in the (t, x)-plane bounded by the lines $x \pm t = 0$ and $x \pm t = 1$. It will then only be possible to prescribe arbitrary boundary conditions along two adjacent sides of the diamond. In [12], it is shown that the image of $\mathbf{d}L_{\partial U}(\varphi)$ will in this case only be isotropic, while for the non-characteristic square the image of $\mathbf{d}L_{\partial U}(\varphi)$ can be shown to be Lagrangian. We will not dwell on the continuous case any further and refer instead to [12, 14], but later on we will see that a similar dichotomy arises in the discrete context.

Maxwell's Equations. We finish with a brief note on the case of field theories with gauge freedom, and we treat electromagnetism as an example. The Lagrangian density for Maxwell's equations is given by

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \tag{3.14}$$

where $F_{\mu\nu}$ is given in terms of the electromagnetic potential A_μ by $F_{\mu\nu} = \partial_\nu A_\mu - \partial_\mu A_\nu$, or in other words, $F = \mathbf{d}A$ when viewed as differential forms. As the Lagrangian does not involve the time derivatives of A_0, it is degenerate, and as a consequence Maxwell's equations, given by $\partial_\mu F^{\mu\nu} = 0$, do not determine A_μ uniquely.

While this might preclude defining the boundary Lagrangian in a straightforward way as in (3.1), we can use the alternative definition (3.4) to introduce $L_{\partial U}$. Note first of all that any two solutions of Maxwell's equations A, A' differ by a gauge transformation, $A' = A + \mathbf{d}f$ for some function f, while the action defined by the Lagrangian (3.14) is gauge invariant: $\mathcal{S}(A) = \mathcal{S}(A + \mathbf{d}f)$. As a result, $\mathcal{S}$ takes on the same value for any solution of Maxwell's equation, so that we can use (3.4) to obtain $L_{\partial U}$ by extremizing $\mathcal{S}$. In differential form notation, we have that

$$\begin{aligned} L_{\partial U}(A) &= \int_U \mathbf{d}A \wedge *\mathbf{d}A \\ &= \int_U \mathbf{d}(A \wedge *\mathbf{d}A) - \int_U A \wedge \mathbf{d} * \mathbf{d}A \\ &= \int_{\partial U} A_{|\partial U} \wedge (*\mathbf{d}A)_{|\partial U}, \end{aligned}$$

where A is a solution of Maxwell's equations in the interior of U, so that $\mathbf{d} * \mathbf{d}A = 0$. On the last line, $A_{|\partial U}$ is the restriction of A to the boundary ∂U, and similarly for $(*\mathbf{d}A)_{|\partial U}$.

One issue now remains: how should the boundary data for A along ∂U be specified? The boundary Lagrangian inherits the gauge freedom of the original Lagrangian density: for all functions f, we have that $L_{\partial U}(A+\mathbf{d}f) = L_{\partial U}(A)$. Secondly, if A and A' are boundary data whose tangential parts agree on ∂U, i.e. such that $A_{|\partial U} = A'_{|\partial U}$, then $L_{\partial U}(A) = L_{\partial U}(A')$. This can be seen by considering the following integral: since $A_{|\partial U} - A'_{|\partial U} = 0$, we have trivially that

$$\int_{\partial U} (A_{|\partial U} - A'_{|\partial U}) \wedge (*\mathbf{d}(A + A'))_{|\partial U} = 0.$$

By expanding the left-hand side we then obtain

$$L_{\partial U}(A) - L_{\partial U}(A') - \int_{\partial U} A'_{|\partial U} \wedge (*\mathbf{d}A)_{|\partial U} + \int_{\partial U} A_{|\partial U} \wedge (*\mathbf{d}A')_{|\partial U} = 0.$$

Through repeated use of Stokes' theorem and the Maxwell equations, the last two terms on the right hand side can be made to vanish, so that we can conclude that $L_{\partial U}(A) = L_{\partial U}(A')$.

As a result, rather than specifying the four-dimensional vector potential $A = A_\mu dx^\mu$ along ∂U, it is sufficient to specify only the tangential part $A_{|\partial U}$. Moreover, since $L_{\partial U}$ is gauge invariant, $L_{\partial U}$ depends only on the equivalence class of $A_{|\partial U}$ under gauge transformations and so we may define a new functional

$$\widehat{L}_{\partial U}(\mathbf{d}A_{|\partial U}) := L_{\partial U}(A_{|\partial U}),$$

where we assume that the topology of ∂U is sufficiently simple, so that we can identify exact two-forms with equivalence classes of one-forms up to exact forms. If ∂U is locally given by $x^0 = 0$, then $\mathbf{d}A_{|\partial U}$ can be identified with the magnetic field B. In general though, $\mathbf{d}A_{|\partial U}$ will contain both electric and magnetic parts relative to the splitting of Minkowski space into space and time, but we conclude that it is sufficient to specify $B := \mathbf{d}A_{|\partial U}$ along ∂U.

4 Type-I/II Generating Functionals

The purpose of this section is to show that the boundary Lagrangian $L_{\partial U}$ can be viewed as a generating functional, in some appropriate sense. We proceed along the following route: first, we take variational derivatives to define a mapping from $\mathcal{Y}_{\partial U}$ to $T^*\mathcal{Y}_{\partial U}$, given by

$$\mathbf{d}L_{\partial U} : \varphi \in \mathcal{Y}_{\partial U} \mapsto \frac{\delta L_{\partial U}}{\delta \varphi}(\varphi) \in T^*\mathcal{Y}_{\partial U}$$

and generated by $L_{\partial U}$. That is, $\mathbf{d}L_{\partial U}(\varphi)$ gives us the normal momenta $\delta L_{\partial U}/\delta\varphi$, given the fields φ at the boundary. Secondly, we show that the image of this map is a Lagrangian submanifold of $T^*\mathcal{Y}_{\partial U}$ with respect to the canonical symplectic structure (2.3). Since $\mathbf{d}L_{\partial U}$ is an exact one-form, this will be a straightforward consequence of the property (2.4). Based on these two properties, we will say that $L_{\partial U}$ is an example of a Type-I generating functional. As an interesting side-result, we obtain that the Lagrangian nature of the image of $\mathbf{d}L_{\partial U}$ is intimately related to the multisymplectic form formula (3.10).

In the second part of this section, we show that the image of $\mathbf{d}L_{\partial U}$ can be generated by other functionals as well. More precisely, we can imagine subdividing the boundary ∂U into two subsets A and B, and prescribing boundary data φ_A along A and normal momenta π_B along B. We can then define a functional $H_{\partial U}(\varphi_A, \pi_B)$ of these data, whose variational derivative with respect to φ_A is the normal momentum along A, and whose variational derivative with respect to π_B is the field φ along B. Consequently, the image of $\mathbf{d}\mathfrak{S}_{\mathrm{II}}$ coincides with the image of $\mathbf{d}H_{\partial U}$ in $T^*\mathcal{Y}_{\partial U}$, and in analogy with mechanics, we will call $H_{\partial U}$ a Type-II generating functional.

Geometry of Generating Functionals. Let $\mathfrak{S} : \mathcal{Y}_{\partial U} \to \mathbb{R}$ be an arbitrary functional on the space of boundary data. The exterior derivative $\mathbf{d}\mathfrak{S}$ is a closed form, and its image is a Lagrangian submanifold of $T^*\mathcal{Y}_{\partial U}$. If instead we restrict $\mathbf{d}\mathfrak{S}$ to a subspace $\mathcal{K}_{\partial U}$ of $T^*\mathcal{Y}_{\partial U}$, the resulting image is no longer Lagrangian, and we obtain merely an isotropic submanifold. We collect these observations in the following theorem, the proof of which is a combination of standard results in symplectic geometry (see, for instance, [1]).

Theorem 4.1. *Let $\mathcal{K}_{\partial U} \subset \mathcal{Y}_{\partial U}$ be a subset of the space of boundary data, let $\mathfrak{S}$ be a functional on $\mathcal{K}_{\partial U}$, and consider the image $\mathcal{M}_{\partial U} := \mathbf{d}\mathfrak{S}(\mathcal{K}_{\partial U})$. Then $\mathcal{M}_{\partial U}$ is an isotropic submanifold of $T^*\mathcal{Y}_{\partial U}$. If $\mathcal{K}_{\partial U} = \mathcal{Y}_{\partial U}$, then $\mathcal{M}_{\partial U}$ is Lagrangian.*

By analogy with mechanics, we refer to any functional $\mathfrak{S}$ on the space of boundary data $\mathcal{Y}_{\partial U}$ as a ***Type-I generating functional***. We now make this analogy more precise. Consider a mechanical system with configuration space Q, and identify the space of boundary data with $Q\times Q$ and the space of normal momenta with $T^*Q\times T^*Q$, equipped with the symplectic form $-\Omega_0 \oplus \Omega_1$, where Ω_i, $i = 0, 1$, is the canonical symplectic form on the ith factor. A function $S(q_0, q_1)$ on $Q \times Q$ then generates a symplectic transformation

$$\left(q_0, \frac{\partial S}{\partial q_0}\right) \mapsto \left(q_1, \frac{\partial S}{\partial q_1}\right)$$

in the standard sense, and our definition is an extension of this concept to classical field theories.

The Boundary Lagrangian as a Type-I Generating Functional. Clearly, the boundary Lagrangian $L_{\partial U} : \mathcal{Y}_{\partial U} \to \mathbb{R}$ is a Type-I generating function in the sense described above. We let $\mathcal{M}_{\partial U}$ be the image of $\mathbf{d}L_{\partial U}$, restricted to the space of admissible boundary conditions $\mathcal{K}_{\partial U}$. We can identify $\mathcal{M}_{\partial U}$ with $\mathcal{K}_{\partial U}$, and under this identification the restriction to $\mathcal{M}_{\partial U}$ of the symplectic form ω on $T^*\mathcal{Y}_{\partial U}$ is given by the pull-back form $(\mathbf{d}L_{\partial U})^*\omega$. From Theorem 4.1, we know that $\mathcal{M}_{\partial U}$ is isotropic, so that this form vanishes. However, some interesting results can be obtained by explicitly writing out $(\mathbf{d}L_{\partial U})^*\omega$ and equating the result with zero.

The canonical symplectic form ω is given by $\omega = -\mathbf{d}\Theta$, where Θ is the canonical one-form on $T^*\mathcal{Y}_{\partial U}$ defined in (2.3). The pullback of Θ along $\mathbf{d}L_{\partial U} : \mathcal{Y}_{\partial U} \to T^*\mathcal{Y}_{\partial U}$ then satisfies $(\mathbf{d}L_{\partial U})^*\Theta = \mathbf{d}L_{\partial U}$ because of (2.4), so that

$$\big((\mathbf{d}L_{\partial U})^*\Theta\big)(\varphi) \cdot \delta\varphi = \mathbf{d}L_{\partial U}(\varphi) \cdot \delta\varphi = \int_{\partial U} (j^1\phi)^* \left(\mathbf{i}_{j^1V}\Theta_L\right),$$

where we have used (3.8). Here, ϕ is again the unique solution of the Euler-Lagrange equations with boundary data φ, and V is a first variation of ϕ induced by the boundary variation $\delta\varphi$. By taking exterior derivatives of both sides and using (3.9), we obtain

$$\big((\mathbf{d}L_{\partial U})^*\omega\big)(\varphi) \cdot (\delta\varphi, \delta\varphi') = \int_{\partial U} (j^1\phi)^* \left(\mathbf{i}_{j^1W}\mathbf{i}_{j^1V}\Omega_L\right), \tag{4.1}$$

but by isotropy, we have that the left-hand side of this formula has to vanish. As a result, we conclude that $\mathcal{M}_{\partial U}$ is isotropic if and only if the multisymplectic form formula (3.10) holds.

The De Donder-Weyl Equations. Given a Lagrangian density $\mathcal{L} = L(x^\mu, y^a, y^a_\mu)\, dV$, we define the multi-momenta p^μ_a (where $a = 1, \ldots, k$, $\mu = 0, \ldots, n$) and a scalar momentum p as

$$p^\mu_a = \frac{\partial L}{\partial y^a_\mu} \quad \text{and} \quad p = L - \frac{\partial L}{\partial y^a_\mu} y^a_\mu. \tag{4.2}$$

These momenta can be defined intrinsically by considering the Legendre transformation as a map from the jet bundle to its extended dual (see, for instance, [6]). We now introduce the Hamiltonian function $\mathcal{H}(x^\mu, y^a, p, p^\mu_a)$ as

$$\mathcal{H}(x^\mu, y^a, p, p^\mu_a) = \operatorname*{ext}_{y^a_\mu} \left[p + p^\mu_a y^a_\mu - L(x^\mu, y^a, y^a_\mu)\right],$$

where we take the extremum over all values of y^a_μ. For a related, coordinate-invariant definition of $\mathcal{H}$, we refer to [2]. Note that $\mathcal{H}$ vanishes identically on the image of the Legendre transformation (4.2), and that L does not necessarily have to hyperregular for $\mathcal{H}$ to be defined.

For the remainder of this paper, we will focus on the locally defined function $H(x^\mu, y^a, p^\mu_a) = p^\mu_a y^a_\mu - L(x^\mu, y^a, y^a_\mu)$, which we will term the ***multi-Hamiltonian (function)***. We emphasize, however, that unlike $\mathcal{H}$, H is in general only locally defined, but all the objects defined in this section can be defined in terms of $\mathcal{H}$ solely.

We now rewrite the action density $\mathcal{S}$ in terms of the Hamiltonian function:

$$\mathcal{S}_H(y^a, p_a^\mu) = \int_U (p_a^\mu y_{,\mu}^a - H(x^\mu, y^a, p_a^\mu))\, d^{n+1}x$$

and we notice that by taking variations of y^a and p_a^μ, we obtain

$$\begin{aligned} D\mathcal{S}_H(y^a, p_a^\mu) \cdot (\delta y^a, \delta p_a^\mu) = \int_U \left(-\left(\frac{\partial p_a^\mu}{\partial x^\mu} + \frac{\partial H}{\partial y^a} \right) \delta y^a + \left(\frac{\partial y^a}{\partial x^\mu} - \frac{\partial H}{\partial p_a^\mu} \right) \delta p_a^\mu \right) d^{n+1}x \\ + \int_{\partial U} p_\mu^a \delta y^a \, d^n x_\mu. \end{aligned} \tag{4.3}$$

Under the condition that the variation δy^a vanish on the boundary ∂U, we obtain the following set of partial differential equations (referred to as the ***De Donder-Weyl equations***):

$$\frac{\partial y^a}{\partial x^\mu} = \frac{\partial H}{\partial p_a^\mu}, \quad \text{and} \quad \frac{\partial p_a^\mu}{\partial x^\mu} = -\frac{\partial H}{\partial y^a}. \tag{4.4}$$

Type-II Generating Functionals. We consider again a fixed domain $U \subset X$ and we divide the boundary ∂U into two disjoint parts A and B: $\partial U = A \cup B$. We suppose that, on A, we are given fixed boundary fields φ_A, while on B we are given fixed normal momenta π_B. We recall that the components of the normal momenta can be expressed as

$$(\pi_B)_a = p_a^\mu \, \iota^*(d^n x_\mu),$$

where $\iota : \partial U \hookrightarrow X$ is the inclusion of the boundary in X.

For given boundary data (φ_A, π_B), let $(\phi^a(x), p_a^\mu(x))$ be the solution of the De Donder-Weyl equations (4.4) with those boundary data, and define the functional

$$\begin{aligned} H_{\partial U}(\varphi_A, \pi_B) &= -\mathcal{S}_H(\phi^a, p_a^\mu) + \int_B (\pi_B) \cdot \phi_{|B} \\ &= -\int_U ({p_a}^\mu \phi_{,\mu}^a - H(\phi^a, {p_a}^\mu))\, d^{n+1}x + \int_B {p_a}^\mu \phi^a \, d^n x_\mu, \end{aligned}$$

which we refer to as the ***boundary Hamiltonian***. We now compute the derivative of $H_{\partial U}$, keeping in mind the boundary conditions, so that $\delta\varphi_{|A} = \delta\pi_{|B} = 0$. A similar computation as for the derivation of (4.3) yields

$$\begin{aligned} DH_{\partial U}(\varphi_A, \pi_B) \cdot (\delta\varphi_A, \delta\pi_B) = \int_U \left(-\left(\frac{\partial p_a^\mu}{\partial x^\mu} + \frac{\partial H}{\partial y^a} \right) \delta y^a + \left(\frac{\partial y^a}{\partial x^\mu} - \frac{\partial H}{\partial p_a^\mu} \right) \delta p_a^\mu \right) d^{n+1}x \\ + \int_B \delta p_a^\mu y^a \, d^n x_\mu - \int_A p_a^\mu \delta y^a \, d^n x_\mu. \end{aligned}$$

The integral over the interior vanishes since (ϕ^a, p_a^μ) is a solution of the De Donder-Weyl equations, and the boundary integrals can be written in terms of the normal momenta as

$$DH_{\partial U}(\varphi_A, \pi_B) \cdot (\delta\varphi_A, \delta\pi_B) = \int_B \delta\pi_B \cdot \phi_{|B} - \int_A \pi_{|A} \cdot \delta\varphi_A,$$

so that the variational derivatives are given by

$$\frac{\delta H_{\partial U}}{\delta \varphi_A} = -\pi_{|A}, \quad \text{and} \quad \frac{\delta H_{\partial U}}{\delta \pi_B} = \phi_{|B}. \tag{4.5}$$

We compare this with the case of mechanical systems. Given a finite time interval $[t_0, t_1]$, a Type-II generating function is a function $S(q_0, p_1)$ depending on the position variables q_0 at the initial time t_0 and on the momenta p_1 at the final time t_1. The final position q_1 and the initial momentum p_0 are then defined by

$$p_0 = \frac{\partial S}{\partial q_0} \quad \text{and} \quad q_1 = \frac{\partial S}{\partial p_1}.$$

The relations (4.5) are the analogue of these expressions for field theory, where the relative minus sign is again due to the orientation of the boundary.

5 Example: Euler Discretization of the Wave Equation

In this section, we show that concepts such as the boundary Lagrangian can also be defined for discrete field theories. Under a few modest assumptions on the discretizations used, we recover, among other things, the discrete multisymplectic form formula of [19]. Throughout this section, we use the Euler discretization of the linear wave Lagrangian as a motivating example. For this special case, we discuss the influence of the geometry of the boundary on the expression for the multisymplectic form formula, and we show that the latter reduces to the multisymplectic conservation law derived by Bridges et al. [3–5]. Our treatment is inspired by the one in [13, 19], where different discretizations and more complex field theories are treated.

For the sake of convenience, we restrict ourselves to a scalar field theory with two independent variables, which we label by t and x. We assume that we are given a regular quadrangular mesh in the base space, with mesh lengths Δt and Δx, and we denote the nodes in this mesh by $(n, i) \in \mathbb{Z} \times \mathbb{Z}$. Note that the node (n, i) corresponds to the point $x_i^n := (n\Delta t, i\Delta x)$ in $\mathbb{R}^2$. We denote the value of the field u at the node (n, i) by u_i^n.

As in [19], we introduce a discrete version of the jet bundle as follows. We define a ***triangle*** at (n, i) to be the ordered triple $((n, i), (n, i + 1), (n + 1, i))$, which we denote by $\triangle_i^n$ (or simply by $\triangle$ if no confusion can arise), and we let $X_\triangle$ be the set of all such triangles.

Given a triangle $\triangle = ((n,i),(n,i+1),(n+1,i))$, we refer to the vertices in a concise way by $\triangle_1 := (n,i)$, $\triangle_2 := (n,i+1)$, and $\triangle_3 := (n+1,i)$.

The discrete jet bundle is then given by (see [19]):

$$J^1_\triangle Y := \{(u_i^n, u_{i+1}^n, u_i^{n+1}) \in \mathbb{R}^3 : ((n,i),(n,i+1),(n+1,i)) \in X_\triangle\},$$

and so is equal to $X_\triangle \times \mathbb{R}^3$. Given an element $(u_i^n, u_{i+1}^n, u_i^{n+1})$ of the discrete jet bundle, we define the triangle midpoint by $\bar{u}_i^n := (u_i^n + u_{i+1}^n + u_i^{n+1})/3$, and we introduce the following first-order expressions for the temporal velocity v_i^n and the spatial velocity w_i^n:

$$v_i^n := \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad \text{and} \quad w_i^n := \frac{u_{i+1}^n - u_i^n}{\Delta x}. \tag{5.1}$$

Consequently, we can discretize a given Lagrangian density L on $J^1 Y$ by

$$L_d(u_i^n, u_{i+1}^n, u_i^{n+1}) := \frac{\Delta t \Delta x}{2} L\left(\frac{u_i^{n+1} - u_i^n}{\Delta t}, \frac{u_{i+1}^n - u_i^n}{\Delta x}, \frac{u_i^n + u_{i+1}^n + u_i^{n+1}}{3}\right). \tag{5.2}$$

For the linear wave equation, with Lagrangian (3.12), the discrete Lagrangian becomes

$$L_d(u_i^n, u_{i+1}^n, u_i^{n+1}) = \frac{\Delta t \Delta x}{4}\left(\left(\frac{u_i^{n+1} - u_i^n}{\Delta t}\right)^2 - \left(\frac{u_{i+1}^n - u_i^n}{\Delta x}\right)^2\right).$$

Poincaré-Cartan Forms. Given a discrete Lagrangian L_d, we introduce the discrete Poincaré-Cartan forms Θ_L^1, Θ_L^2 and Θ_L^3 by

$$\Theta_L^1(u_i^n, u_{i+1}^n, u_i^{n+1}) := D_1 L_d(u_i^n, u_{i+1}^n, u_i^{n+1})\, du_i^n,$$

and similarly for Θ_L^2 and Θ_L^3. Note that these forms are one-forms on the discrete jet bundle, and that $\Theta_L^1 + \Theta_L^2 + \Theta_L^3 = \mathbf{d}L$. Furthermore, we put $\Omega_L^k = -\mathbf{d}\Theta_L^k$ (for $k = 1,2,3$), so that

$$\Omega_L^1 + \Omega_L^2 + \Omega_L^3 = 0. \tag{5.3}$$

For the linear wave equation, a straightforward computation yields

$$\Omega_L^1 = \frac{1}{2}((\Delta x)\, dv_i^n \wedge du_i^n - (\Delta t)\, dw_i^n \wedge du_i^n) \tag{5.4}$$

as well as

$$\Omega_L^2 = \frac{1}{2}(\Delta t)\, dw_i^n \wedge du_i^n, \quad \text{and} \quad \Omega_L^3 = -\frac{1}{2}(\Delta x)\, dv_i^n \wedge du_i^n, \tag{5.5}$$

where v_i^n and w_i^n are given by (5.1).

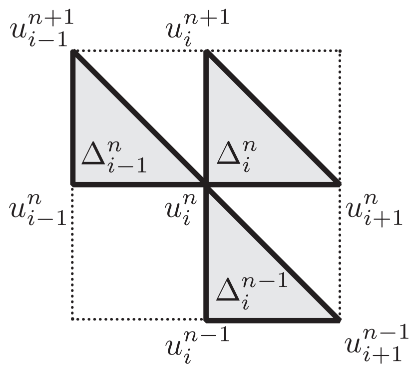

Figure 1: Three adjacent triangles touching a common vertex, labeled by u_i^n.

Discrete Euler-Lagrange Equations. Given a finite subset $U \subset X_\triangle$ of the space of triangles, we form the ***discrete action sum*** as

$$\mathcal{S}_U(u) := \sum_{\triangle \in U} L_d(j^1 u(\triangle)).$$

Here, u is a ***discrete field***, assigning to every node (n, i) a field value u_i^n, and $j^1 u$ is its ***first jet extension***, defined by

$$(j^1 u)(\triangle) = (u(\triangle_1), u(\triangle_2), u(\triangle_3)) \in J^1_\triangle Y.$$

We now focus on a particular configuration U, consisting of three adjacent triangles, as in Figure 1. The action sum for this U is explicitly given by

$$\mathcal{S}_U(u) = L_d(u_i^n, u_{i+1}^n, u_i^{n+1}) + L_d(u_{i-1}^n, u_i^n, u_{i-1}^{n+1}) + L_d(u_i^{n-1}, u_{i+1}^{n-1}, u_i^n). \tag{5.6}$$

By keeping the values of the field on the boundary fixed, and taking variations with respect to $u_{n,i}$, we obtain the following ***discrete Euler-Lagrange equations***:

$$D_1 L_d(u_i^n, u_{i+1}^n, u_i^{n+1}) + D_2 L_d(u_{i-1}^n, u_i^n, u_{i-1}^{n+1}) + D_3 L_d(u_i^{n-1}, u_{i+1}^{n-1}, u_i^n) = 0. \tag{5.7}$$

We can rewrite these equations in terms of the discrete Poincaré-Cartan forms as

$$\Theta_L^1(\triangle_i^n) + \Theta_L^2(\triangle_{i-1}^n) + \Theta_L^3(\triangle_i^{n-1}) = 0, \tag{5.8}$$

where $\triangle_i^n$, etc., refer to the triangles defined in Figure 1.

For the wave equation (3.12), the discrete Euler-Lagrange equations result in the standard second-order scheme

$$-\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta t)^2} + \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} = 0. \tag{5.9}$$

Discrete Boundary Lagrangian. We now mimic the construction in Section 3 to introduce a discrete version of the boundary Lagrangian. We refer again to Figure 1 and we define the boundary Lagrangian to be the extremal value of the action sum (5.6), taking variations over the interior node u_i^n. For the sake of notation, we denote the values of the field on the boundary by $u_{\partial U}$, so that

$$u_{\partial U} := (u_{i+1}^n, u_i^{n+1}, u_{i-1}^{n+1}, u_{i-1}^n, u_i^{n-1}, u_{i+1}^{n-1}).$$

The boundary Lagrangian is then given by

$$L_{\partial U}(u_{\partial U}) := \operatorname*{ext}_{u_i^n} \big[L_d(u_i^n, u_{i+1}^n, u_i^{n+1}) + L_d(u_{i-1}^n, u_i^n, u_{i-1}^{n+1}) + L_d(u_i^{n-1}, u_{i+1}^{n-1}, u_i^n) \big], \quad (5.10)$$

where the extremum is taken over all u_i^n. Alternatively, $L_{\partial U}$ can be defined by solving the discrete Euler-Lagrange equations (5.7) for u_i^n given the values of $u_{\partial U}$ as boundary data, and substituting this value into the action sum (5.6).

Discrete Multisymplectic Form Formula. We now derive the discrete multisymplectic form formula by twice taking the exterior derivative of the boundary Lagrangian $L_{\partial U}$. By taking the exterior derivative of both sides of (5.10) and using the definition of the Poincaré-Cartan forms given above, we obtain

$$\mathbf{d}L_{\partial U} = \sum_{k=1}^{3} \sum_{l=1}^{3} \Theta_L^k(\Delta^{(l)}).$$

Using the discrete Euler-Lagrange equations (5.8), we can rewrite this as

$$\mathbf{d}L_{\partial U} = \sum_{k=1}^{3} \sum_{l=1; l\neq k}^{3} \Theta_L^k(\Delta^{(l)}), \quad (5.11)$$

and by taking another exterior derivative of both sides, and using that $\mathbf{d}^2 L_{\partial U} \equiv 0$, we finally obtain

$$0 = \sum_{k=1}^{3} \sum_{l=1; l\neq k}^{3} \Omega_L^k(\Delta^{(l)}). \quad (5.12)$$

This is precisely the multisymplectic form formula derived in [19], applied to the triangular domain of Figure 1. For the linear wave equation, we can substitute the expressions (5.4) and (5.5) for the discrete multisymplectic forms to obtain

$$\frac{1}{\Delta x}(dw_i^n \wedge du_i^n - dw_{i-1}^n \wedge du_{i-1}^n) - \frac{1}{\Delta t}(dv_i^n \wedge du_i^n - dv_i^{n-1} \wedge du_i^{n-1}) = 0.$$

This is the multisymplectic conservation law of Bridges and Reich [4] applied to the linear wave equation, but we caution against taking this result too far: in general the discrete Euler-Lagrange equations (5.7) will be different from the discrete multisymplectic equations of Bridges and Reich. Consequently, the discrete multisymplectic form formula (5.12) will also lead to different multisymplectic conservation laws.

Lagrangian Submanifolds and Characteristics. With the notations of the previous paragraph, let $\mathcal{M}_{\partial U}$ be the image of $\mathbf{d}L_{\partial U}$ given by (5.11). Note that $\mathcal{M}_{\partial U}$ is a submanifold of $(T^*Q)^{\times 6}$, where we have one copy of T^*Q for each boundary point in Figure 1. Note that $\mathcal{M}_{\partial U}$ is the image of an exact one-form, and hence determines at least an isotropic submanifold of $(T^*Q)^{\times 6}$. If there are no extra conditions on the boundary data, then $\mathcal{M}_{\partial U}$ will be Lagrangian.

We now discuss the relation between the location of the boundary data and the nature of $\mathcal{M}_{\partial U}$. To keep the computations to a minimum, we restrict ourselves to the linear wave equation. We first solve the discrete wave equations (5.9) to determine u_i^n in terms of the boundary data. The discrete wave equation can be rewritten as

$$2(c^2-1)u_i^n = c^2(u_{i+1}^n + u_{i-1}^n) - (u_i^{n+1} + u_i^{n-1}) \tag{5.13}$$

where $c := \Delta t/\Delta x$ is the aspect ratio of the mesh. If the CFL condition is satisfied, so that $c < 1$, this expression can be used to determine u_i^n in terms of the boundary data. However, when $c = 1$, the left-hand side vanishes and we merely obtain a relation between the boundary data. In this case, the boundary data are located on characteristics of the continuous wave equation.

As a result, whenever the boundary data is characteristic, there exist supplementary compatibility conditions between the boundary data, and hence $\mathcal{M}_{\partial U}$ is strictly isotropic. When the boundary is noncharacteristic, there are no further conditions on the data and $\mathcal{M}$ is Lagrangian. We outlined a similar result for the continuous wave equation at the end of Section 3.

6 Conclusion and Future Directions

In this paper, we consider the space of boundary data for a Lagrangian field theory, whose tangent space is the space of Cauchy data, and we introduce a duality pairing between the space of Cauchy data and normal momenta. We then introduce the boundary Lagrangian, which is the analogue of Jacobi's solution of the Hamilton–Jacobi equation, and consider more generally the concept of Type-I and Type-II generating functionals for a Lagrangian field theory.

We are interested in the following topics for future work:

- *Continuous and Discrete Hamilton–Jacobi Theory for Field Theories.* By computing variations of Jacobi's solution of the Hamilton–Jacobi equation, one can recover the Hamilton–Jacobi equation. In a similar way, we intend to use the concept of the boundary Lagrangian to systematically derive a Hamilton–Jacobi equation for covariant field theories.

In [21], a discrete Jacobi's solution was used to derive a discrete Hamilton–Jacobi equation, which is in turn related to the Hamilton–Jacobi–Bellman equation of optimal control. It would be interesting to develop the analogous connection between discrete Hamilton–Jacobi theory for fields and numerical methods for the optimal boundary control of Lagrangian field theories.

- *Variational Error Analysis of Variational Integrators for Field Theories.* Since the boundary Lagrangian $L_{\partial U}$ and the boundary Hamiltonian $H_{\partial U}$ are exact generating functionals for Lagrangian and Hamiltonian field theories, it would be natural to extend the theory of variational error analysis introduced in [18] to the setting of discrete field theories, and to develop general techniques for constructing variational integrators for field theories by extending the approaches for constructing Lagrangian and Hamiltonian variational integrators described in [15, 16].

- *Connections with Multisymplectic Integrators for Hamiltonian PDEs.* A variational characterization of discrete multisymplectic variational integrators for Hamiltonian field theories is a natural direction to pursue, and will involve a combination of the insights developed in this paper, and a generalization of the methods developed in [16]. The goal would be to provide a systematic characterization of the associated discrete multisymplectic conservation laws, and appropriate invariance properties of the discrete Hamiltonian which would lead to a discrete multisymplectic Noether's theorem. This connections between such a discrete variational approach and the multisymplectic integrators described in [4, 5] remain to be elucidated.

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