MULTISYMPLECTIC HAMILTONIAN VARIATIONAL INTEGRATORS

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Abstract. Variational integrators have traditionally been constructed from the perspective of Lagrangian mechanics, but there have been recent efforts to adopt discrete variational approaches to the symplectic discretization of Hamiltonian mechanics using Hamiltonian variational integrators. In this paper, we will extend these results to the setting of Hamiltonian multisymplectic field theories. We demonstrate that one can use the notion of Type II generating functionals for Hamiltonian partial differential equations as the basis for systematically constructing Galerkin Hamiltonian variational integrators that automatically satisfy a discrete multisymplectic conservation law, and establish a discrete Noether's theorem for discretizations that are invariant under a Lie group action on the discrete dual jet bundle. In addition, we demonstrate that for spacetime tensor product discretizations, one can recover the multisymplectic integrators of Bridges and Reich, and show that a variational multisymplectic discretization of a Hamiltonian multisymplectic field theory using spacetime tensor product Runge–Kutta discretizations is well-defined if and only if the partitioned Runge–Kutta methods are symplectic in space and time.

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1. Introduction

Variational integrators have become an important class of geometric numerical integrators for the simulation of mechanical systems, and provides a systematic method of constructing symplectic

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integrators. The variational approach has numerous benefits, the first of which is that the resulting numerical integrators are automatically symplectic, and if they are group-invariant, then they satisfy a discrete Noether's theorem and preserve a discrete momentum map. In addition, it can be shown that the order of accuracy is related to the best approximation properties of the finite-dimensional function spaces and the order of the quadrature rule used to construct the variational integrator [15].

However, the variational integrator approach has traditionally been applied to Lagrangian formulations of mechanical systems, as summarized in Marsden and West [27], and the development of Hamiltonian variational integrators has been less extensive. The notion of Hamiltonian variational integrators was first introduced in Lall and West [21] as the dual formulation of a discrete constrained variational principle, but it did not provide an explicit characterization of the discrete Hamiltonian in terms of the continuous Hamiltonian and the corresponding discrete Noether's theorem, which was introduced in Leok and Zhang [24]. This involves constructing the exact Type II/Type III generating functions for the Hamiltonian flow of a mechanical system, which can be viewed as the analogue of Jacobi's solution of the Hamilton–Jacobi equation. The variational error analysis result for Hamiltonian variational integrators was established in Schmitt and Leok [36], and methods based on Taylor expansions were developed in Schmitt et al. [37].

Hamiltonian variational integrators also find application in discrete optimal control and discrete Hamilton–Jacobi theory, and it was shown in Ohsawa et al. [31] that the Bellman equations of discrete optimal control are the lowest order approximation of a continuous optimal control problem arising from a particular choice of Hamiltonian variational integrator. The Poincaré transformed Hamiltonian was used independently by Hairer [13] and Reich [32] as a means of constructing time-adaptive symplectic integrators, and an adaptive approach based on Hamiltonian variational integrators was developed in Duruisseaux et al. [10]. The Hamiltonian approach is necessary in this case as many monitor functions result in Poincaré transformed Hamiltonians that are degenerate, for which no Lagrangian analogue exists.

In the setting of Lagrangian and Hamiltonian partial differential equations, multisymplectic integrators that can be viewed as generalizations of symplectic integrators for mechanical systems to field theories were introduced from a Lagrangian perspective in Marsden et al. [28], and from the Hamiltonian, but non-variational perspective, in Bridges and Reich [6]. Our approach to constructing a variational description of multisymplectic integrators for Hamiltonian partial differential equations is based on the notion of generating functionals for multisymplectic relations that was introduced in Vankerschaver et al. [39].

The advantage of the discrete variational principle approach is that it automatically yields multisymplectic integrators, and exhibit a discrete analogue of Noether's theorem. Furthermore, they naturally lend themselves to Galerkin discretizations that allow for the systematic construction of multisymplectic integrators by choosing a finite-dimensional approximation space for sections of the configuration bundle, and a numerical quadrature rule. In addition, group-invariant discretizations that exhibit a discrete Noether's theorem can be constructed from finite-dimensional approximation spaces that are equivariant with respect to the Lie symmetry group that generates the relevant momentum map.

1.1. **Lagrangian and Hamiltonian Variational Integrators.**

Geometric numerical integration aims to preserve geometric conservation laws under discretization, and this field is surveyed in the monograph by Hairer et al. [14]. Discrete variational mechanics [23; 27] provides a systematic method of constructing symplectic integrators. It is typically approached from a Lagrangian perspective by introducing the *discrete Lagrangian*, $L_d : Q \times Q \to \mathbb{R}$, which is a Type I generating function of a symplectic map and approximates the *exact discrete Lagrangian*,

$$L_d^E(q_0, q_1; h) = \operatorname{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t)) dt, \tag{1.1}$$

which is equivalent to Jacobi's solution of the Hamilton–Jacobi equation. The exact discrete Lagrangian generates the exact discrete-time flow map of a Lagrangian system, but, in general, it cannot be computed explicitly. Instead, this can be approximated by replacing the integral with a quadrature formula, and replacing the space of C^2 curves with a finite-dimensional function space. Given a finite-dimensional function space $\mathbb{M}^n([0,h]) \subset C^2([0,h],Q)$ and a quadrature formula $\mathcal{G} : C^2([0,h],Q) \to \mathbb{R}$, $\mathcal{G}(f) = h \sum_{j=1}^m b_j f(c_j h) \approx \int_0^h f(t)dt$, the *Galerkin discrete Lagrangian* is

$$L_d(q_0, q_1) = \operatorname{ext}_{\substack{q \in \mathbb{M}^n([0,h]) \\ q(0)=q_0, q(h)=q_1}} \mathcal{G}(L(q, \dot{q})) = \operatorname{ext}_{\substack{q \in \mathbb{M}^n([0,h]) \\ q(0)=q_0, q(h)=q_1}} h \sum_{j=1}^m b_j L(q(c_j h), \dot{q}(c_j h)).$$

Given a discrete Lagrangian L_d, the *discrete Hamilton–Pontryagin principle* imposes the discrete second-order condition $q_k^1 = q_{k+1}^0$ using Lagrange multipliers p_{k+1}, which yields a variational principle on $(Q \times Q) \times_Q T^*Q$,

$$\delta \left[\sum_{k=0}^{n-1} L_d(q_k^0, q_k^1) + \sum_{k=0}^{n-2} p_{k+1}(q_{k+1}^0 - q_k^1) \right] = 0.$$

This in turn yields the *implicit discrete Euler–Lagrange equations*,

$$q_k^1 = q_{k+1}^0, \qquad p_{k+1} = D_2 L_d(q_k^0, q_k^1), \qquad p_k = -D_1 L_d(q_k^0, q_k^1), \tag{1.2}$$

where D_i denotes the partial derivative with respect to the i-th argument. Making the identification $q_k = q_k^0 = q_{k-1}^1$, we obtain the *discrete Lagrangian map* and *discrete Hamiltonian map* which are $F_{L_d} : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ and $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, respectively. The last two equations of (1.2) define the *discrete fiber derivatives*, $\mathbb{F}L_d^{\pm} : Q \times Q \to T^*Q$,

$$\mathbb{F}L_d^+(q_k, q_{k+1}) = (q_{k+1}, D_2 L_d(q_k, q_{k+1})),$$
$$\mathbb{F}L_d^-(q_k, q_{k+1}) = (q_k, -D_1 L_d(q_k, q_{k+1})).$$

These two discrete fiber derivatives induce a single unique *discrete symplectic form*, $\Omega_{L_d} = (\mathbb{F}L_d^{\pm})^* \Omega$, and the discrete Lagrangian and Hamiltonian maps preserve Ω_{L_d} and Ω, respectively. The discrete Lagrangian and Hamiltonian maps can be expressed as $F_{L_d} = (\mathbb{F}L_d^-)^{-1} \circ \mathbb{F}L_d^+$ and $\tilde{F}_{L_d} = \mathbb{F}L_d^+ \circ (\mathbb{F}L_d^-)^{-1}$, respectively. This characterization allows one to relate the approximation error of the discrete flow maps to the approximation error of the discrete Lagrangian.

The variational integrator approach simplifies the numerical analysis of symplectic integrators. The task of establishing the geometric conservation properties and order of accuracy of the discrete Lagrangian map F_{L_d} and discrete Hamiltonian map $\tilde{F}_{L_d}$ reduces to the simpler task of verifying certain properties of the discrete Lagrangian L_d instead.

Theorem 1.1 (Discrete Noether's theorem (Theorem 1.3.3 of [27]))**.** *If a discrete Lagrangian L_d is invariant under the diagonal action of G on $Q \times Q$, then the single unique discrete momentum map, $\mathbf{J}_{L_d} = (\mathbb{F}L_d^{\pm})^* \mathbf{J}$, is invariant under the discrete Lagrangian map F_{L_d}, i.e., $F_{L_d}^* \mathbf{J}_{L_d} = \mathbf{J}_{L_d}$.*

Theorem 1.2 (Variational error analysis (Theorem 2.3.1 of [27]))**.** *If a discrete Lagrangian L_d approximates the exact discrete Lagrangian L_d^E to order p, i.e., $L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) + \mathcal{O}(h^{p+1})$, then the discrete Hamiltonian map $\tilde{F}_{L_d}$ is an order p accurate one-step method.*

The bounded energy error of variational integrators can be understood by performing backward error analysis, which then shows that the discrete flow map is approximated with exponential accuracy by the exact flow map of the Hamiltonian vector field of a modified Hamiltonian [4; 38].

Given a degenerate Hamiltonian, where the Legendre transform $\mathbb{F}H : T^*Q \to TQ$, $(q,p) \mapsto (q, \frac{\partial H}{\partial p})$, is noninvertible, there is no equivalent Lagrangian formulation. Thus, a characterization of variational integrators directly in terms of the continuous Hamiltonian is desirable. This is achieved by considering the Type II analogue of Jacobi's solution, given by

$$H_d^{+,E}(q_k, p_{k+1}) = \operatorname{ext}_{\substack{(q,p)\in C^2([t_k,t_{k+1}],T^*Q)\\ q(t_k)=q_k, p(t_{k+1})=p_{k+1}}} \left[p(t_{k+1})q(t_{k+1}) - \int_{t_k}^{t_{k+1}} [p\dot{q} - H(q,p)]\, dt \right].$$

A computable Galerkin discrete Hamiltonian H_d^+ is obtained by choosing a finite-dimensional function space and a quadrature formula,

$$H_d^+(q_0, p_1) = \operatorname{ext}_{\substack{q\in\mathbb{M}^n([0,h])\\ q(0)=q_0\\ (q(c_jh),p(c_jh))\in T^*Q}} \left[p_1 q(t_1) - h \sum\nolimits_{j=1}^m b_j [p(c_jh)\dot{q}(c_jh) - H(q(c_jh), p(c_jh))] \right].$$

Interestingly, the Galerkin discrete Hamiltonian does not require a choice of a finite-dimensional function space for the curves in the momentum, as the quadrature approximation of the action integral only depend on the momentum values $p(c_jh)$ at the quadrature points, which are determined by the extremization principle. In essence, this is because the action integral does not depend on the time derivative of the momentum $\dot{p}$. As such, both the Galerkin discrete Lagrangian and the Galerkin discrete Hamiltonian depend only on the choice of a finite-dimensional function space for curves in the position, and a quadrature rule. It was shown in Proposition 4.1 of [24] that when the Hamiltonian is hyperregular, and for the same choice of function space and quadrature rule, they induce equivalent numerical methods.

The *Type II discrete Hamilton's phase space variational principle* states that

$$\delta \left\{ p_N q_N - \sum_{k=0}^{N-1} \left[p_{k+1}q_{k+1} - H_d^+(q_k, p_{k+1}) \right] \right\} = 0,$$

for discrete curves in T^*Q with fixed (q_0, p_N) boundary conditions. This yields the *discrete Hamilton's equations*, which are given by

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \qquad p_k = D_1 H_d^+(q_k, p_{k+1}). \tag{1.3}$$

Given a discrete Hamiltonian H_d^+, we introduce the *discrete fiber derivatives* (or discrete Legendre transforms), $\mathbb{F}^+ H_d^+$,

$$\begin{aligned} \mathbb{F}^+ H_d^+ &: (q_0, p_1) \mapsto (D_2 H_d^+(q_0, p_1), p_1), \\ \mathbb{F}^- H_d^+ &: (q_0, p_1) \mapsto (q_0, D_1 H_d^+(q_0, p_1)). \end{aligned}$$

The discrete Hamiltonian map can be expressed in terms of the discrete fiber derivatives,

$$\tilde{F}_{H_d^+}(q_0, p_0) = \mathbb{F}^+ H_d^+ \circ (\mathbb{F}^- H_d^+)^{-1}(q_0, p_0) = (q_1, p_1),$$

Similar to the Lagrangian case, we have a discrete Noether's theorem and variational error analysis result for Hamiltonian variational integrators.

Theorem 1.3 (Discrete Noether's theorem (Theorem 5.3 of [24]))**.** *Let Φ^{T^*Q} be the cotangent lift action of the action Φ on the configuration manifold Q. If the generalized discrete Lagrangian $R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1)$ is invariant under the cotangent lifted action Φ^{T^*Q}, then the discrete Hamiltonian map $\tilde{F}_{H_d^+}$ preserves the momentum map, i.e., $\tilde{F}_{H_d^+}^* \mathbf{J} = \mathbf{J}$.*

Theorem 1.4 (Variational error analysis (Theorem 2.2 of [36]))**.** *If a discrete Lagrangian H_d^+ approximates the exact discrete Hamiltonian $H_d^{+,E}$ to order p, i.e., $H_d^+(q_0, p_1; h) = H_d^{+,E}(q_0, p_1; h) + \mathcal{O}(h^{p+1})$, then the discrete Hamiltonian map $\tilde{F}_{H_d^+}$ is an order p accurate one-step method.*

It should be noted that there is an analogous theory of discrete Hamiltonian variational integrators based on Type III generating functions $H_d^-(p_0, q_1)$.

1.2. **Multisymplectic Hamiltonian Field Theory.** While classical field theories can be viewed as an infinite-dimensional Hamiltonian system with time as the independent variable (see, for example, Abraham and Marsden [1]), we will adopt the multisymplectic formulation with spacetime as the independent variables, which has been extensively studied in, for example, Gotay et al. [11, 12], Marsden and Shkoller [26], Marsden et al. [29]. The description of multisymplectic classical field theories in the literature is traditionally formulated in the Lagrangian setting or in the Hamiltonian setting via the covariant Legendre transform to pass between the two settings. However, as we are interested in constructing variational integrators purely within the Hamiltonian setting, we will outline the necessary ingredients of multisymplectic Hamiltonian field theory in this section, without the use of the Lagrangian framework or the covariant Legendre transform.

Consider a trivial vector bundle $E = X \times Q \to X$ over an oriented spacetime X (although we will refer to X as spacetime with evolutionary Hamiltonian PDEs in mind, X could be either Riemannian or Lorentzian), with volume form denoted $d^{n+1}x$. Let Θ be the Cartan form on the dual jet bundle J^1E^*, which has coordinates $(x^\mu, \phi^A, p, p^A_\mu)$, where x^μ are the coordinates on spacetime, ϕ^A are the coordinates on Q, and p and p^A_μ are the coordinates of the affine map on the jet bundle, $v^A_\mu \mapsto (p + p^\mu_A v^A_\mu)d^{n+1}x$. Define the restricted dual jet bundle $\widetilde{J^1E^*}$ as the quotient of J^1E^* by horizontal one-forms; this space is coordinatized by (x^μ, ϕ^A, p^A_μ) and is the relevant configuration bundle for a Hamiltonian field theory; we interpret ϕ^A as the value of the field and p^μ_A as the associated momenta in the direction x^μ. The dual jet bundle can be viewed as a bundle over the restricted bundle, $\mu : J^1E^* \to \widetilde{J^1E^*}$ (see León et al. [25]). Let $H \in C^\infty(\widetilde{J^1E^*})$ be the Hamiltonian of our theory. This defines a section of μ, in coordinates $\tilde{H}(x^\mu, \phi^A, p^\mu_A) = (x^\mu, \phi^A, -H, p^\mu_A)$ or using the projections $\pi^{j,k}$ from the bundle of $(j + k)$-forms on E to the subbundle of j-horizontal, k-vertical forms, this can be defined as the set of $z \in J^1E^*$ such that $\pi^{n+1,0}(z) = -H(\pi^{n,1}(z))d^{n+1}x$. Using this section, one can pullback the Cartan form to a form on the restricted bundle,

$$\Theta_H = \tilde{H}^*\Theta = p^\mu_A d\phi^A \wedge d^n x_\mu - H d^{n+1}x.$$

We then define the action S^U (relative to an arbitrary region $U \subset X$) as a functional on the sections of $\widetilde{J^1E^*}$ (viewed as a bundle over spacetime),

$$S^U[\phi, p] = \int_U (\phi, p)^*\Theta_H. \tag{1.4}$$

Hamilton's principle states that this action is stationary for compactly supported vertical variations, i.e.,

$$0 = dS^U[\phi, p] \cdot V = \int_U (\phi, p)^* i_V d\Theta_H + \underbrace{\int_{\partial U} (\phi, p)^* i_V \Theta_H}_{=0,\ V \Subset U}.$$

Since U is arbitrary, for a sufficiently smooth solution, this gives the strong form of Hamilton's equations, $(\phi, p)^* i_V \Omega_H = 0$, where we defined the multisymplectic form $\Omega_H = -d\Theta_H$. In coordinates, for $V = \delta\phi^A \partial/\partial\phi^A + \delta p^\mu_A \partial/\partial p^\mu_A$, these equations read

$$\delta\phi^A(\partial_\mu p^\mu_A + \frac{\partial H}{\partial\phi^A})d^{n+1}x + \delta p^\mu_A(-\partial_\mu\phi^A + \frac{\partial H}{\partial p^\mu_A})d^{n+1}x = 0.$$

Since this must hold for $\delta\phi^A, \delta p^\mu_A$ independent, this gives the De Donder–Weyl equations

$$\partial_\mu p^\mu_A = -\frac{\partial H}{\partial\phi^A}, \tag{1.5a}$$

$$\partial_\mu\phi^A = \frac{\partial H}{\partial p^\mu_A}. \tag{1.5b}$$

To write these equations as a multi-Hamiltonian system, define $z^A = (\phi^A, p^0_A, \dots, p^n_A)^T$; it is clear that the De Donder–Weyl equations can be written as

$$\underbrace{\begin{pmatrix} 0 & -1 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}}_{\equiv K^0} \partial_0 z^A + \dots + \underbrace{\begin{pmatrix} 0 & 0 & \dots & 0 & -1 \\ 0 & \ddots & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}}_{\equiv K^n} \partial_n z^A = \nabla_{z^A} H,$$

or $K^0\partial_0 z^A + \dots + K^n\partial_n z^A = \nabla_{z^A} H$, where the matrices K^μ are $(n+2)\times(n+2)$ skew-symmetric matrices which have value -1 in the $(0, \mu+1)$ entry and 1 in the $(\mu+1, 0)$ entry (we are indexing the matrices from 0 to $n+1$), and 0 everywhere else. This form of the equations was studied in Bridges [5]. We can associate to each of these matrices a degenerate two-form,

$$\omega^\mu \equiv \sum_A d(z^A)^T \otimes K^\mu dz^A = (-dp^\mu_A \otimes d\phi^A + d\phi^A \otimes dp^\mu_A) = d\phi^A \wedge dp^\mu_A.$$

For simplicity of notation, we will implicitly suppress the duality pairing between $(\phi^A)_A$ (valued in Q) and $(p^\mu_A)_A$ (valued in Q^*) and write this as $\omega^\mu = d\phi \wedge dp^\mu$ (throughout, we will suppress this duality pairing, e.g. $p^\mu\phi \equiv p^\mu_A\phi^A$). Hamilton's equations $(\phi, p)^* i_V \Omega_H = 0$ can then be written as $\omega^\mu(\partial_\mu z, V) = 0$ (sum over μ), which relates the multisymplectic structure Ω_H to $(n+1)$-presymplectic structures $\{\omega^\mu\}$.

Remark 1.1. *Of course, the multisymplectic structure is more fundamental, since the ω^μ were constructed via a particular coordinate representation. Since we will utilize Cartesian coordinates on a rectangular mesh for discretization, these coordinate representatives will be simpler to deal with and correspond to the current literature on multisymplectic integrators; however, for discretizations on spaces that do not admit global coordinates, utilizing the multisymplectic structure is more fundamental and in principle, the method for constructing variational integrators that we will describe can be used in this more general setting.*

Multisymplecticity and the Boundary Hamiltonian. The above Hamiltonian system admits a notion of conserving multisymplecticity, which generalizes the usual notion of symplecticity. In particular, let V, W be two first variations, i.e., vector fields whose flows map solutions of Hamilton's equations again to solutions; then, for any region $U \subset X$, one has the multisymplectic form formula:

$$\int_{\partial U} (\phi, p)^*(i_V i_W \Omega_H) = 0, \tag{1.6}$$

which follows from $d^2 S^U[\phi,p]\cdot(V,W)=0$ for a solution (ϕ,p) of Hamilton's equations. In coordinates where $V=\delta\phi^A\partial/\partial\phi^A+\delta p^\mu_A\partial/\partial p^\mu_A$ and $V=\delta y^A\partial/\partial\phi^A+\delta\pi^\mu_A\partial/\partial p^\mu_A$, this reads

$$0=\int_{\partial U}(\phi,p)^*(i_V i_W\Omega_H)=\int_{\partial U}(\delta\phi^A\delta\pi^\mu_A-\delta y^A\delta p^\mu_A)|_{(\phi,p)}d^nx_\mu=\int_{\partial U}\omega^\mu|_{(\phi,p)}(V,W)d^nx_\mu.$$

Applying Stokes' theorem and noting that U is arbitrary, the strong form of the multisymplectic form formula can be expressed $\partial_\mu\omega^\mu=0$, which holds when evaluated on two first variations at a solution of Hamilton's equations (ϕ,p). In terms of our coordinate representation of Hamilton's equations, by taking the exterior derivative of Hamilton's equations, a first variation is a vector field V which satisfies

$$K^0dz_0(V)+\cdots+K^ndz_n(V)=(D_{zz}H)dz(V),$$

where $z_\mu\equiv\partial_\mu z$. One of the aims of this paper is to construct variational integrators for multi-Hamiltonian PDEs which admit a discrete analog of the multisymplectic conservation law for a suitably defined discrete notion of first variations.

Analogous to how the Type II generating functions are utilized in the construction of Galerkin Hamiltonian variational integrators (see Leok and Zhang [24]), we will utilize the boundary Hamiltonian introduced in Vankerschaver et al. [39], which will act as a generalized Type II generating functional. Consider a domain $U\subset X$ and partition the boundary $\partial U=A\cup B$; we supply fixed field boundary values φ_A on A and fixed normal momenta π_B on B. The boundary Hamiltonian is defined as a functional on these boundary values

$$\begin{aligned}H_{\partial U}(\varphi_A,\pi_B)&=\text{ext}\Big[\int_B p^\mu\phi d^nx_\mu-\int_U(\phi,p)^*\Theta_H\Big]\\&=\text{ext}\Big[\int_B p^\mu\phi d^nx_\mu-\int_U(p^\mu\partial_\mu\phi-H(\phi,p))d^{n+1}x\Big],\end{aligned}\tag{1.7}$$

where one extremizes over all fields (ϕ,p) satisfying the fixed boundary conditions along A and B. This is a Type II generating functional in the sense that it generates the boundary values for the field along B (denoted $\phi|_B$) and the normal momenta along A (denoted $p^n|_A$),

$$\frac{\delta H_{\partial U}}{\delta\varphi_A}=-p^n|_A,\quad\frac{\delta H_{\partial U}}{\delta\pi_B}=\phi|_B.\tag{1.8}$$

Note that the generating relation (1.8) only determines the normal component of the momentum along A; this is consistent with the De Donder–Weyl equation (1.5a), since it only specifies $\partial_\mu p^\mu$.

Since we are extremizing over the fields (ϕ,p) which satisfy the boundary conditions, they are of course the solutions to Hamilton's equation and thus satisfy the multisymplectic form formula. Since the multisymplectic form formula is expressed as an integral over ∂U and the generating functional gives us the field values on ∂U, $(\varphi,\pi)=(\varphi_A,\varphi_B,\pi_A,\pi_B)$, the above generating map (1.8) is multisymplectic in the sense

$$\int_{\partial U}\omega^\mu|_{(\varphi,\pi)}(V,W)d^nx_\mu=0,$$

for first variations V and W.

We will utilize a discrete approximation of the boundary Hamiltonian and its property as a generating functional to construct variational integrators which are naturally multisymplectic.

Noether's Theorem. Another important conservative property of Hamiltonian systems arises from symmetries. Suppose there is a smooth group action of G on the restricted dual jet bundle which leaves the action S^U invariant. Let $\tilde{\xi}$ denote the infinitesimal generator vector field for $\xi \in \mathfrak{g}$ associated to this action. For a solution (ϕ, p) of Hamilton's equations, one has

$$0 = \pounds_{\tilde{\xi}} S^U[\phi, p] = dS^U[\phi, p] \cdot \tilde{\xi} = \int_U (\phi, p)^* i_{\tilde{\xi}} d\Theta_H + \int_{\partial U} (\phi, p)^* i_{\tilde{\xi}} \Theta_H.$$

Note that the term involving the integral over U vanishes, even though $\tilde{\xi}$ is not necessarily compactly supported in U, since Hamilton's equations hold pointwise (U is arbitrary). Hence, Noether's theorem in this setting is the statement

$$\int_{\partial U} (\phi, p)^* i_{\tilde{\xi}} \Theta_H = 0. \tag{1.9}$$

In the discrete setting, we will be particularly concerned with vertical variations (where the group action on the base space X is the identity). In this case, we can write the above in coordinates as

$$\int_{\partial U} p^\mu (i_{\tilde{\xi}} d\phi) d^n x_\mu = 0. \tag{1.10}$$

We will see that if there is a group action on the discrete analog of the restricted dual jet bundle which leaves the discrete action (the generalized discrete Lagrangian) invariant, then there is a discrete analog of Noether's theorem, equation (1.10).

1.3. **Multisymplectic Integrators for Hamiltonian PDEs.** Consider the class of Hamiltonian PDEs,

$$K^0 z_0 + \cdots + K^n z_n = \nabla_z H(z), \tag{1.11}$$

with independent variable $x = (x^0, \dots, x^n) \in \mathbb{R}^{n+1}$, dependent variable $z : \mathbb{R}^n \to \mathbb{R}^m$, each K^μ is an $m \times m$ skew-symmetric matrix, and the Hamiltonian $H : \mathbb{R}^m \to \mathbb{R}$ is sufficiently smooth.

Defining a two-form for each K^μ, $\omega^\mu(U, V) = \langle K^\mu U, V \rangle$ (with respect to an inner product $\langle \cdot, \cdot \rangle$ on $\mathbb{R}^m$), the equation (1.11) admits the multisymplectic conservation law

$$\partial_\mu \omega^\mu(U, V) = 0, \tag{1.12}$$

for any pair of first variations U, V satisfying the variational equation

$$K^0 dz_0 + \cdots + K^n dz_n = D_{zz} H(z).$$

As we saw, the De Donder–Weyl equations, which arose from the variational principle applied to the Hamiltonian action (1.4), are an example of a Hamiltonian PDE in the form (1.11). From our variational perspective, the action and variational principle are more fundamental, as opposed to the field equations (1.11). However, as shown by **?**], the Hamiltonian system (1.11) arises from the variational principle, so there is no loss of generality working with the formulation based on the Hamiltonian action (1.4).

For the Hamiltonian system (1.11), a multisymplectic integrator is defined in Bridges and Reich [6] to be a method

$$K^0 \partial_0^{i_0 \dots i_n} z_{i_0 \dots i_n} + \cdots + K^n \partial_n^{i_0 \dots i_n} z_{i_0 \dots i_n} = (\nabla_z S(z_{i_0 \dots i_n}))_{i_0 \dots i_n},$$

where $\partial_\mu^{i_0 \dots i_n}$ is a discretization of ∂_μ, such that a discrete analog of equation (1.12) holds,

$$\partial_\mu^{i_0 \dots i_n} \omega^\mu(U_{i_0 \dots i_n}, V_{i_0 \dots i_n}) = 0,$$

when evaluated on discrete first variations $U_{i_0 \dots i_n}, V_{i_0 \dots i_n}$ satisfying the discrete variational equations

$$K^0 \partial_0^{i_0 \dots i_n} dz_{i_0 \dots i_n} + \cdots + K^n \partial_n^{i_0 \dots i_n} dz_{i_0 \dots i_n} = d\Big((\nabla_z S(z_{i_0 \dots i_n}))_{i_0 \dots i_n} \Big).$$

We will see that the variational integrators that we construct will automatically satisfy a discrete multisymplectic conservation law, as a consequence of the Type II variational principle. Furthermore, we will show in Section 2.4 that this discrete multisymplectic conservation law reproduces the Bridges and Reich notion of multisymplecticity.

Example 1.1. *An example of a multisymplectic integrator in* $1+1$ *spacetime dimensions is the centered Preissman scheme,*

$$K^0 \frac{z^1_{1/2} - z^0_{1/2}}{\Delta t} + K^1 \frac{z^{1/2}_1 - z^{1/2}_0}{\Delta x} = \nabla_z H\Big(z^{1/2}_{1/2}\Big),$$

where $z^0_{1/2} = \frac{1}{2}(z^0_0 + z^0_1)$, *etc. and* $z^{1/2}_{1/2} = \frac{1}{4}(z^1_1 + z^0_1 + z^1_0 + z^0_0)$. *As noted in Reich [34], this can be obtained from a cell-vertex finite volume discretization on a rectangular grid, or alternatively, as observed in Reich [33], it is an example of a multisymplectic Gauss–Legendre collocation method, in the case of one collocation point. Furthermore, the multisymplectic Gauss–Legendre collocation methods are members of a larger class of multisymplectic integrators, the multisymplectic partitioned Runge–Kutta methods (see, for example, Hong et al. [18], Ryland et al. [35]). In Section 2.3, we will derive the class of multisymplectic partitioned Runge–Kutta methods within our variational framework.*

2. Multisymplectic Hamiltonian Variational Integrators

2.1. **Discrete Hamiltonian Field Theory.** We will discuss our construction of a discrete boundary Hamiltonian for the general case of an arbitrary mesh and subsequently study the particular case of a rectangular mesh where the variational equations can be written explicitly. Let $X \subset \mathbb{R}^{n+1}$ be a polygonal domain and $\mathcal{T}(X)$ an associated mesh. In general, a discrete configuration bundle consists of a choice of finite element space taking values in the fiber Q that is subordinate to the mesh $\mathcal{T}(X)$. To be more concrete, for every mesh element $\triangle \in \mathcal{T}(X)$, we introduce nodes $x_i \in \triangle, i \in I$, and parametrize the finite element space by the fiber value at each node. A multisymplectic variational integrator based on finite elements was developed from the Lagrangian perspective in Chen [9].

The discrete analog of the configuration bundle, on an element by element level, is the base space $\{x_i\}_{i\in I}$ with fiber Q over each node; the total space is $\{x_i\}_{i\in I} \times Q$ and a section is a map from each node to Q, denoted $\phi_i \in Q$. Analogously, the discrete analog of the restricted dual jet bundle is $\{x_i\}_{i\in I} \times Q \times (Q^*)^{n+1}$, where a section is specified by $\phi_i \in Q, p^\mu_i \in Q^*$. Let $S^\triangle_d[\phi_i, p^\mu_i]$ be some discrete approximation of the action $S^\triangle[\phi, p]$. As in the discussion of the boundary Hamiltonian (1.7), partition the boundary of the element $\partial\triangle = A \cup B$ and let $\displaystyle\sum\!\!\!\!\!\!\int_B \pi_B\varphi_B$ be some discrete approximation to the boundary integral $\int_B p^\mu \phi d^n x_\mu$, depending only on the field and normal momenta boundary values on the nodes $x_i \in B$, which we denoted φ_B and π_B respectively. Define the discrete boundary Hamiltonian

$$H^{\partial\triangle}_d(\varphi_A, \pi_B) = \operatorname*{ext}_{\substack{\phi_i \in Q, p^\mu_i \in Q^* \\ \phi|_A = \varphi_A, p^n|_B = \pi_B}} \Big[\sum\!\!\!\!\!\!\!\int \pi_B\varphi_B - S^\triangle_d[\phi_i, p^\mu_i] \Big],$$

where $p^n|_B$ denotes the normal component of the momenta along B. Repeat the above construction for each $\triangle \in \mathcal{T}(X)$; partitioning the boundaries $\partial\triangle = A(\triangle) \cup B(\triangle)$ and the boundary of the full region $\partial X = A(X) \cup B(X)$ (where $A(X) = \cup_{\Delta\in\mathcal{T}(X)}(A(\Delta) \cap \partial X)$ and $B(X) = \cup_{\Delta\in\mathcal{T}(X)}(B(\Delta) \cap \partial X)$). Define the discrete action sum

$$S_d[\{\varphi_{A(\triangle)}, \pi_{B(\triangle)}\}_{\triangle\in\mathcal{T}(X)}] = \sum\!\!\!\!\!\!\!\int_{B(X)} \pi_{B(X)}\varphi_{B(X)} - \sum_{\triangle\in\mathcal{T}(X)} \Big[\sum\!\!\!\!\!\!\!\int_{B(\triangle)} \pi_{B(\triangle)}\varphi_{B(\triangle)} - H^{\partial\triangle}_d(\varphi_A, \pi_B) \Big].$$

The Type II variational principle $\delta S_d = 0$ (subject to variations of φ vanishing along $A(X)$ and variations of π vanishing along $B(X)$) gives a set of (generally coupled) maps $(\varphi_{A(\triangle)}, \pi_{B(\triangle)}) \mapsto (\varphi_{B(\triangle)}, \pi_{A(\triangle)})$ in analogy with the generating functional relation, equation (1.8). In the case of finite element spaces which are not parametrized by the nodal values, we evaluate the discrete boundary Hamiltonian on the discrete space of boundary data induced by the choice of mesh and discrete configuration bundle, and extremize the expressions above over the finite elements that satisfy the prescribed boundary conditions. This is the most general form of our multisymplectic Hamiltonian variational integrator.

Now, consider the particular case of a rectangular domain X and an associated rectangular mesh $\mathcal{T}(X)$. For simplicity and clarity in the notation, we will focus on the case of $1+1$ spacetime dimensions, although higher dimensions can be treated similarly (as we will see, our method is based on a tensor product quadrature construction; for higher dimensions, just append indices as necessary).

Consider a rectangle $[t, t+\Delta t] \times [x, x+\Delta x] = \square \in \mathcal{T}(X)$. Introduce nodes on the intervals $\{t_1 = t, t_2, \dots, t_{s-1}, t_s = t+\Delta t\}$ and $\{x_1 = x, x_2, \dots, x_{\sigma-1}, x_\sigma = x+\Delta x\}$ (as we will introduce in the next section for Galerkin Hamiltonian variational integrators, these nodes correspond to quadrature points along the time and space intervals). The discrete base space is $X_d = \{(t_i, x_j) \mid i = 1, \dots, s,\ j = 1, \dots, \sigma\}$, the discrete configuration bundle is $X_d \times Q$, where a section is map from each node (t_i, x_j) to (t_i, x_j, ϕ_{ij}), where $\phi_{ij} \in Q$. Analogously, the discrete restricted dual jet bundle is $X_d \times Q \times (Q^*)^2$, where a section is specified by $\phi_{ij} \in Q, p^\mu_{ij} \in Q^*$. Let $S^\square_d[\phi_{ij}, p^\mu_{ij}]$ be some discrete approximation to $S^\square[\phi, p]$ (we will explicitly construct such a discrete approximation in the next section using Galerkin techniques and quadrature). Partitioning the boundary $\partial\square = A(\square) \cup B(\square)$, the discrete boundary Hamiltonian is given by

$$H_d^{\partial\square}(\varphi_{A(\square)}, \pi_{B(\square)}) = \operatorname*{ext}_{\substack{\phi_{ij} \in Q, p^\mu_{ij} \in Q^* \\ \phi|_{A(\square)} = \varphi_{A(\square)}, p^n|_{B(\square)} = \pi_{B(\square)}}} \Big[\sum\!\!\!\!\!\!\int_{B(\square)} \pi_{B(\square)} \varphi_{B(\square)} - S^\square_d[\phi_{ij}, p^\mu_{ij}] \Big], \tag{2.1}$$

where $\varphi_{A(\square)}$ denotes the boundary values on $A(\square)$, i.e., at nodes $(t_i, x_j) \in A$ (and similarly for π). The discrete action sum is

$$S_d\big[\{\varphi_{A(\square)}, \pi_{B(\square)}\}_{\square \in \mathcal{T}(X)}\big] = \sum\!\!\!\!\!\!\int_{B(X)} \pi_{B(X)} \varphi_{B(X)} - \sum_{\square \in \mathcal{T}(X)} \Big[\sum\!\!\!\!\!\!\int_{B(\square)} \pi_{B(\square)} \varphi_{B(\square)} - H_d^{\partial\square}(\varphi_{A(\square)}, \pi_{B(\square)}) \Big].$$

Recall the Type II variational principle $\delta S_d = 0$ gives a set of maps $(\varphi_{A(\square)}, \pi_{B(\square)}) \mapsto (\varphi_{B(\square)}, \pi_{A(\square)})$. To give a more explicit characterization of these maps, let us introduce a quadrature approximation of the boundary integral over B. First, consider the simple case of one quadrature point along each edge of $\square_{ab} = [t_0 + a\Delta t, t_0 + (a+1)\Delta t] \times [x_0 + b\Delta x, x_0 + (b+1)\Delta x]$, where $\mathcal{T}(X) = \{\square_{ab}\}_{a,b}$. Let $\varphi_{[a]b}$ denote the field boundary value at the quadrature point along the bottom edge $(t_a, t_a + \Delta t) \times \{x_b\}$ (where we orient our axes such that time is horizontal and space is vertical) and $\varphi_{a[b]}$ denote its value at the quadrature point along the left edge $\{t_a\} \times (x_b, x_b + \Delta x)$ (and similarly $\varphi_{[a]b+1}$ for the top edge, $\varphi_{a+1[b]}$ for the right edge). We take A to be the bottom and left edges, and B to the top and right edges. The normal momenta through the top edge is the momenta associated to the x direction (at the quadrature point), which we denote $\pi^1_{[a]b+1}$, and the normal momenta through the right edge is the momenta associated to the t direction, which we denote $\pi^0_{a+1[b]}$. Since we only have one quadrature point along each edge, the quadrature weight for the temporal edge is Δt and similarly for the spatial edge is Δx. See Figure 1.

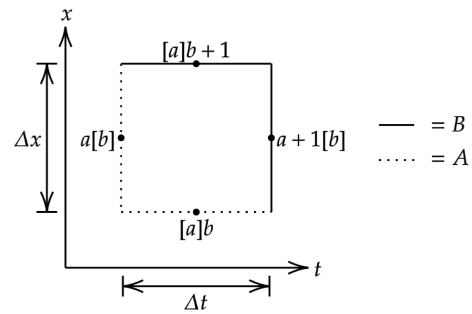

FIGURE 1. Schematic for one quadrature point along each edge of $\square_{ab} \in \mathcal{T}(X)$.

Then, the boundary integral can be approximated

$$\begin{aligned}\int_B p^\mu \phi d^n x_\mu &= \int_{t_a}^{t_{a+1}} (p^1\phi)|_{x=x_{b+1}} dt + \int_{x_b}^{x_{b+1}} (p^0\phi)_{t=t_{a+1}} dx \\ &\approx \pi^1_{[a]b+1}\varphi_{[a]b+1}\Delta t + \pi^0_{a+1[b]}\varphi_{a+1[b]}\Delta x \equiv \sum_B \pi_B \varphi_B.\end{aligned}$$

The associated discrete boundary Hamiltonian is

$$H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}) = \text{ext}\left(\pi^1_{[a]b+1}\varphi_{[a]b+1}\Delta t + \pi^0_{a+1[b]}\varphi_{a+1[b]}\Delta x - S_d^{\square_{ab}}[\phi, p]\right),$$

where the $+$ specifies that we chose B to be in the forward direction (in the direction of increasing temporal and spatial values), analogous to the notion of discrete right Hamiltonian in discrete mechanics. Again, we extremize over ϕ, p satisfying the boundary conditions (note we have not given an explicit construction for such a $S_d^{\square_{ab}}$ yet; see Section 2.2).

Proposition 2.1. *The Type II variational principle $\delta S_d = 0$, subject to variations of φ vanishing along $A(X)$ and variations of π vanishing along $B(X)$, yields the following,*

$$\pi^1_{[a]b} = \frac{1}{\Delta t} D_1 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2a}$$

$$\pi^0_{a[b]} = \frac{1}{\Delta x} D_2 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2b}$$

$$\varphi_{[a]b+1} = \frac{1}{\Delta t} D_3 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2c}$$

$$\varphi_{a+1[b]} = \frac{1}{\Delta x} D_4 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}), \tag{2.2d}$$

where D_i denotes differentiation with respect to the i^{th} argument. We refer to these equations as the discrete forward Hamilton's equations (in the case of one quadrature point). Note that these equations define a map $(\varphi_A, \pi_B) = (\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}) \mapsto (\varphi_B, \pi_A) = (\phi_{[a]b+1}, \phi_{a+1[b]}, \pi^1_{[a]b}, \pi^0_{a[b]})$.

Proof. Recall the full mesh $\mathcal{T}(X) = \{\square_{ab}\}_{a,b}$; say $a = 0, \dots, N-1$, and $b = 0, \dots, M-1$ (so that $X = [t_0, t_0 + N\Delta t] \times [x_0, x_0 + M\Delta x]$). $B(X)$ consists of the forward edges of X, i.e.,

$$B(X) = \Big([t_0, t_0 + N\Delta t] \times \{x_0 + M\Delta x\}\Big) \cup \Big(\{t_0 + N\Delta t\} \times [x_0, x_0 + M\Delta x]\Big).$$

Consider the discrete action sum

$$S_d[\{\varphi_{A(\square)}, \pi_{B(\square)}\}]$$

$$
\begin{aligned}
&= \sum\!\!\!\!\!\!\int_{B(X)} \pi_{B(X)}\varphi_{B(X)} - \sum_{\square\in\mathcal{T}(X)} \Big[\sum\!\!\!\!\!\!\int_{B(\square)} \pi_{B(\square)}\varphi_{B(\square)} - H_d^+(\varphi_{A(\square)}, \pi_{B(\square)}) \Big] \\
&= \sum_{a=0}^{N-1} \pi^1_{[a]M}\varphi_{[a]M}\Delta t + \sum_{b=0}^{M-1} \pi^0_{N[b]}\varphi_{N[b]}\Delta x \\
&\quad - \sum_{a,b=0}^{N-1,M-1} \Big[\pi^1_{[a]b+1}\varphi_{[a]b+1}\Delta t + \pi^0_{a+1[b]}\varphi_{a+1[b]}\Delta x - H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]}) \Big] \\
&= \underbrace{- \sum_{a,b=0}^{N-1,M-2} \pi^1_{[a]b+1}\varphi_{[a]b+1}\Delta t}_{\equiv(a)} \underbrace{- \sum_{a,b=0}^{N-2,M-1} \pi^0_{a+1[b]}\varphi_{a+1[b]}\Delta x}_{\equiv(b)} \\
&\quad \underbrace{+ \sum_{a,b=0}^{N-1,M-1} H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})}_{\equiv(c)} .
\end{aligned}
$$

The Type II variational principle states $0 = \delta S_d = \delta(a) + \delta(b) + \delta(c)$, subject to variations of φ vanishing along $A(X)$ (i.e., $\delta\varphi_{[a]0} = 0 = \delta\varphi_{0[b]}$) and variations of π vanishing along $B(X)$ (i.e., $\delta\pi^0_{N[b]} = 0 = \delta\pi^1_{[a]M}$). Compute the variations of $(a), (b), (c)$ keeping only the independent variations $\delta\varphi_{[a]b}$, $\delta\varphi_{a[b]}$, $\delta\pi^0_{a[b]}$, $\delta\pi^1_{[a]b}$ not required to vanish by the boundary conditions (note such vanishing variations will only appear in (c)).

$$
\begin{aligned}
\delta(a) &= -\Delta t \sum_{a=0}^{N-1}\sum_{b=0}^{M-2} \Big(\varphi_{[a]b+1}\delta\pi^1_{[a]b+1} + \pi^1_{[a]b+1}\delta\varphi_{[a]b+1} \Big) \\
&= -\Delta t \sum_{a=0}^{N-1}\sum_{b=0}^{M-2} \varphi_{[a]b+1}\delta\pi^1_{[a]b+1} - \Delta t \sum_{a=0}^{N-1}\sum_{b=1}^{M-1} \pi^1_{[a]b}\delta\varphi_{[a]b}, \\
\delta(b) &= -\Delta x \sum_{a=0}^{N-2}\sum_{b=0}^{M-1} \Big(\varphi_{a+1[b]}\delta\pi^0_{a+1[b]} + \pi^0_{a+1[b]}\delta\varphi_{a+1[b]} \Big) \\
&= -\Delta x \sum_{a=0}^{N-2}\sum_{b=0}^{M-1} \varphi_{a+1[b]}\delta\pi^0_{a+1[b]} - \Delta x \sum_{a=1}^{N-1}\sum_{b=0}^{M-1} \pi^0_{a[b]}\delta\varphi_{a[b]}.
\end{aligned}
$$

For brevity, denote $H_d^+[a,b] \equiv H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})$. Compute

$$
\begin{aligned}
\delta(c) = &\sum_{a,b=0}^{N-1,M-1} \Big(D_1H_d^+[a,b]\delta\varphi_{[a]b} + D_2H_d^+[a,b]\delta\varphi_{a[b]} + D_3H_d^+[a,b]\delta\pi^1_{[a]b+1} + D_4H_d^+[a,b]\delta\pi^0_{a+1[b]} \Big) \\
&= \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_1H_d^+[a,b]\delta\varphi_{[a]b} + \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_2H_d^+[a,b]\delta\varphi_{a[b]} \\
&\quad + \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_3H_d^+[a,b]\delta\pi^1_{[a]b+1} + \sum_{a=0}^{N-1}\sum_{b=0}^{M-1} D_4H_d^+[a,b]\delta\pi^0_{a+1[b]}.
\end{aligned}
$$

Note in the first double sum above, $\delta\varphi_{[a]0} = 0$ so we remove the $b = 0$ terms. In the second double sum, $\delta\varphi_{0[b]} = 0$ so we remove the $a = 0$ terms. In the third double sum above, $\delta\pi^1_{[a]M} = 0$ so we remove the $b = M - 1$ terms. In the fourth double sum above, $\delta\pi^0_{N[b]} = 0$ so we remove the $a = N - 1$ terms. This gives,

$$\begin{aligned}\delta(c) = &\sum_{a=0}^{N-1}\sum_{b=1}^{M-1} D_1 H_d^+[a,b]\delta\varphi_{[a]b} + \sum_{a=1}^{N-1}\sum_{b=0}^{M-1} D_2 H_d^+[a,b]\delta\varphi_{a[b]} \\ &+ \sum_{a=0}^{N-1}\sum_{b=0}^{M-2} D_3 H_d^+[a,b]\delta\pi^1_{[a]b+1} + \sum_{a=0}^{N-2}\sum_{b=0}^{M-1} D_4 H_d^+[a,b]\delta\pi^0_{a+1[b]}.\end{aligned}$$

Putting everything together, we have

$$\begin{aligned}0 &= \delta S_d = \delta(a) + \delta(b) + \delta(c) \\ &= \sum_{a=0}^{N-1}\sum_{b=1}^{M-1}(-\Delta t\ \pi^1_{[a]b} + D_1 H_d^+[a,b])\delta\varphi_{[a]b} + \sum_{a=1}^{N-1}\sum_{b=0}^{M-1}(-\Delta x\ \pi^0_{a[b]} + D_2 H_d^+[a,b])\delta\varphi_{a[b]} \\ &\quad + \sum_{a=0}^{N-1}\sum_{b=0}^{M-2}(-\Delta t\ \varphi_{[a]b+1} + D_3 H_d^+[a,b])\delta\pi^1_{[a]b+1} + \sum_{a=0}^{N-2}\sum_{b=0}^{M-1}(-\Delta x\ \varphi_{a+1[b]} + D_4 H_d^+[a,b])\delta\pi^0_{a+1[b]}.\end{aligned}$$

The variations in the above expression are all independent, so this gives (2.2a)-(2.2d). □

Discrete Multisymplecticity. Analogous to the continuum case, we define a discrete first variation as a vector field such that the above equations (2.2a)-(2.2d) still hold when evaluated at the level of the exterior derivative, e.g. for equation (2.2a),

$$d\pi^1_{[a]b} = \frac{1}{\Delta t} d\Big(D_1 H_d^+(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})\Big).$$

and similarly for the others. As we saw in the continuum theory, the map generated by the boundary Hamiltonian implies the multisymplectic form formula, since the multisymplectic form formula can be expressed over the boundary ∂U. Since we constructed a discrete approximation to the boundary Hamiltonian before enforcing the variational principle, we would naturally expect a discrete notion of multisymplecticity to arise as well. Furthermore, in the continuum theory, multisymplecticity follows from $d^2 = 0$ applied to the boundary Hamiltonian, evaluated on first variations. As we will see, our discrete multisymplectic form formula follows from computing $d^2 = 0$ applied to the discrete boundary Hamiltonian, in analogy with the continuum theory.

Proposition 2.2. *The discrete forward Hamilton's equations (2.2a)-(2.2d) are multisymplectic, in the sense that for a solution of the discrete forward Hamilton's equations,*

$$\Delta t\ d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} - \Delta t\ d\varphi_{[a]b} \wedge d\pi^1_{[a]b} + \Delta x\ d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} - \Delta x\ d\varphi_{a[b]} \wedge d\pi^0_{a[b]} = 0,$$

evaluated on discrete first variations.

Proof. In what follows, H_d^+ will be evaluated at $(\varphi_{[a]b}, \varphi_{a[b]}, \pi^1_{[a]b+1}, \pi^0_{a+1[b]})$. Compute

$$\begin{aligned}0 = d^2 H_d^+ &= d\Big(D_1 H_d^+ d\varphi_{[a]b} + D_2 H_d^+ d\varphi_{a[b]} + D_3 H_d^+ d\pi^1_{[a]b+1} + D_4 H_d^+ d\pi^0_{a+1[b]}\Big) \\ &= d(D_1 H_d^+) \wedge d\varphi_{[a]b} + d(D_2 H_d^+) \wedge d\varphi_{a[b]} + d(D_3 H_d^+) \wedge d\pi^1_{[a]b+1} + d(D_4 H_d^+) \wedge d\pi^0_{a+1[b]}.\end{aligned}$$

Then, by our definition of discrete first variations, we have

$$\begin{aligned}d(D_1 H_d^+) &= \Delta t\ d\pi^1_{[a]b}, \\ d(D_2 H_d^+) &= \Delta x\ d\pi^0_{a[b]}, \\ d(D_3 H_d^+) &= \Delta t\ d\varphi_{[a]b+1},\end{aligned}$$

$$d(D_4 H_d^+) = \Delta x \; d\varphi_{a+1[b]}.$$

Substituting these expressions into the equation for $d^2 H_d^+$ yields

$$\begin{aligned}
0 &= d(D_1 H_d^+) \wedge d\varphi_{[a]b} + d(D_2 H_d^+) \wedge d\varphi_{a[b]} + d(D_3 H_d^+) \wedge d\pi^1_{[a]b+1} + d(D_4 H_d^+) \wedge d\pi^0_{a+1[b]} \\
&= \Delta t \; d\pi^1_{[a]b} \wedge d\varphi_{[a]b} + \Delta x \; d\pi^0_{a[b]} \wedge d\varphi_{a[b]} + \Delta t \; d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} + \Delta x \; d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} \\
&= -\Delta t \; d\varphi_{[a]b} \wedge d\pi^1_{[a]b} - \Delta x \; d\varphi_{a[b]} \wedge d\pi^0_{a[b]} + \Delta t \; d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} + \Delta x \; d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} \\
&= \Delta t \; d\varphi_{[a]b+1} \wedge d\pi^1_{[a]b+1} - \Delta t \; d\varphi_{[a]b} \wedge d\pi^1_{[a]b} + \Delta x \; d\varphi_{a+1[b]} \wedge d\pi^0_{a+1[b]} - \Delta x \; d\varphi_{a[b]} \wedge d\pi^0_{a[b]}.
\end{aligned}$$

□

Remark 2.1. *Recall that $\omega^\mu = d\varphi \wedge d\pi^\mu$. Observe that if we divide the above discrete multisymplectic form formula by $\Delta t \Delta x$, it is just a first-order finite difference approximation of $\partial_\mu \omega^\mu = 0$.*

Furthermore, it is clear that the above equation is precisely quadrature applied to the multisymplectic form formula $\int_{\partial \square} \omega^\mu|_{(\varphi,\pi)}(\cdot,\cdot) d^n x_\mu = 0$.

General Quadrature Approximation. From here, the generalization to multiple quadrature points is straight-forward. For simplicity, we take the bottom-left vertex of $\square \in \mathcal{T}(X)$ to be $(0,0)$. Then, $\square = [0,\Delta t] \times [0,\Delta x]$. In the temporal direction, introduce quadrature points $c_i \in [0,1]$, $i = 1,\dots,s$, and associated quadrature weights b_i; we normalize these such that $\sum_i b_i = 1$ (for both c_i and b_i, we'll have to explicitly include a factor of Δt later) and without loss of generality, we assume each $b_i \neq 0$. Similarly, for the spatial direction, introduce quadrature points $\tilde{c}_\alpha$, $\alpha = 1,\dots,\sigma$ and the associated non-zero weights $\tilde{b}_\alpha$ (normalized as before). Let $\varphi_{[i]0} = \varphi(c_i \Delta t, 0)$, $\varphi_{0[\alpha]} = (0, \tilde{c}_\alpha \Delta x)$, $\varphi_{[i]1} = \varphi(c_i \Delta t, \Delta x)$, $\varphi_{1[\alpha]} = (\Delta t, \tilde{c}_\alpha \Delta x)$. Similarly define $\pi^0_{0[\alpha]}$, $\pi^1_{[i]0}$, $\pi^0_{1[\alpha]}$, $\pi^1_{[i]1}$. As before, we take B to be the part of the boundary in the forward direction. See Figure 2.

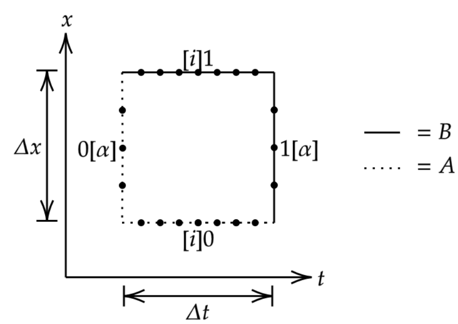

FIGURE 2. Schematic for multiple quadrature points along each edge of $\square \in \mathcal{T}(X)$.

Then, use quadrature to approximate the boundary integral:

$$\begin{aligned}
\int_B p^\mu \phi d^n x_\mu &= \int_0^{\Delta t} (p^1 \phi)|_{x=\Delta x} dt + \int_0^{\Delta x} (p^0 \phi)_{t=\Delta t} dx \\
&\approx \sum_{i=1}^{s} \Delta t \; b_i \pi^1_{[i]1} \varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x \tilde{b}_\alpha p^0_{1[\alpha]} \varphi_{1[\alpha]} \equiv \sum_B\!\!\!\!\!\!\int \pi_B \varphi_B.
\end{aligned}$$

The associated discrete boundary Hamiltonian is

$$H_d^+(\{\varphi_{[i]0}, \varphi_{0[\alpha]}, \pi^1_{[i]1}, \pi^0_{1[\alpha]}\}_{i,\alpha}) = \operatorname{ext}\Big(\sum_{i=1}^{s} \Delta t \; b_i \pi^1_{[i]1} \varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x \tilde{b}_\alpha \pi^0_{1[\alpha]} \varphi_{1[\alpha]} - S_d^{\square_{ab}}[\phi, p] \Big).$$

Proposition 2.3. *The discrete forward Hamilton's equations arising from the Type II variational principle are*

$$\pi^1_{[i]0} = \frac{1}{b_i \Delta t} D_{1,i} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad i = 1, \dots, s, \tag{2.3a}$$

$$\pi^0_{0[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} D_{2,\alpha} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad \alpha = 1, \dots, \sigma, \tag{2.3b}$$

$$\varphi_{[i]1} = \frac{1}{b_i \Delta t} D_{3,i} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad i = 1, \dots, s, \tag{2.3c}$$

$$\varphi_{1[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} D_{4,\alpha} H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}), \qquad \alpha = 1, \dots, \sigma, \tag{2.3d}$$

where $D_{1,i} \equiv \partial/\partial\varphi_{[i]0}$, $D_{2,\alpha} \equiv \partial/\partial\varphi_{0[\alpha]}$, $D_{3,i} \equiv \partial/\partial\pi^1_{[i]1}$, $D_{4,\alpha} \equiv \partial/\partial\pi^0_{1[\alpha]}$. Furthermore, a solution of the discrete forward Hamilton's equations (2.3a)-(2.3d) satisfies the discrete multisymplectic conservation law,

$$\sum_{i=1}^{s} \Delta t \; b_i \Big(d\varphi_{[i]1} \wedge d\pi^1_{[i]1} - d\varphi_{[i]0} \wedge d\pi^1_{[i]0} \Big) + \sum_{\alpha=1}^{\sigma} \Delta x \; \tilde{b}_\alpha \Big(d\varphi_{1[\alpha]} \wedge d\pi^0_{1[\alpha]} - d\varphi_{0[\alpha]} \wedge d\pi^0_{0[\alpha]} \Big) = 0, \tag{2.4}$$

evaluated on discrete first variations.

Proof. The proof follows similarly to the case of one quadrature point, Proposition 2.1. Namely, the discrete forward Hamilton's equations follow from the Type II variational principle $\delta S_d = 0$ subject to variations of φ vanishing along $A(X)$ and variations of π vanishing along $B(X)$. The discrete multisymplectic conservation law follows from

$$d^2 H_d^+(\{\varphi_{[j]0}, \varphi_{0[\beta]}, \pi^1_{[j]1}, \pi^0_{1[\beta]}\}_{j,\beta}) = 0.$$

□

As in the case of one quadrature point, the discrete multisymplectic conservation law is the given quadrature rule applied to $\int_{\partial\Box} \omega^\mu|_{(\varphi,\pi)}(\cdot,\cdot) d^n x_\mu = 0$.

Remark 2.2. *The above discrete forward Hamilton's equations were defined on $\Box = [0, \Delta t] \times [0, \Delta x]$. For $\Box_{ab} = [t_a, t_a + \Delta t] \times [x_b, x_b + \Delta x]$, shift the indices $0, 1$ appropriately to $a, a+1$ and $b, b+1$, i.e., $\varphi_{[i]0} \to \varphi_{[i]b}$, $\varphi_{[i]1} \to \varphi_{[i]b+1}$, $\varphi_{0[\alpha]} \to \varphi_{a[\alpha]}$, $\varphi_{1[\alpha]} \to \varphi_{a+1[\alpha]}$ and similarly for the momenta.*

Boundary Conditions and Solution Method. Recall that the discrete forward Hamilton's equations produce a map $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ for each $\Box \in \mathcal{T}(X)$. However, depending on the boundary conditions that we supply on ∂X, the actual realization of these maps may be different (in that the boundary conditions determine the variables in $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ that we implicitly solve for). The key point is that we must specify the field value or the normal momenta along four edges (and the edges may repeat, such as supplying field values and normal momenta on the same edge; see the discussion of evolutionary systems below). This will depend on whether the Hamiltonian PDE we are considering is stationary or evolutionary.

Consider a stationary system (e.g. an elliptic system). Then, along ∂X, we can specify either Dirichlet boundary conditions, given by the field value φ, or Neumann boundary conditions, given by the normal momenta value π. If we supply such boundary conditions, then each $\Box \in \mathcal{T}(X)$ either has two edges with supplied boundary conditions (those on the corners of X), has one edge with supplied boundary conditions (those on the edges of X), or no supplied boundary conditions (those on the interior). However, the field values and normal momenta values have to be the same along interior edges, which makes up the other required degrees of freedom (recall, we need to specify the field value or normal momenta along four edges). This couples all of the implicit maps $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ together, so that the solution must be solved simultaneously for every $\Box \in \mathcal{T}(X)$. See Figure 3.

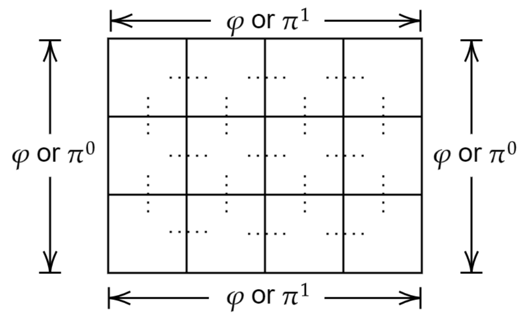

FIGURE 3. Coupling of all of the discrete forward Hamilton's equations for stationary Hamiltonian PDEs; dashed lines along interior edges denote field and normal momenta continuity.

For an evolutionary system (e.g. a hyperbolic system), we specify the initial conditions at $t = 0$, which consist of both the field and normal momenta value (π^0). On the spatial boundaries, we can either supply Dirichlet or Neumann conditions as above. The continuity of field and normal momenta on the interior edges couples the maps $(\varphi_{A(\Box)}, \pi_{B(\Box)}) \mapsto (\varphi_{B(\Box}, \pi_{A(\Box)})$ together for each $\Box$ in the same time slice and produces the remaining required degrees of freedom. Hence, one solves these coupled equations on the first time slice which supplies new initial conditions for the subsequent timeslice; one then continues this process recursively for each time step, thereby allowing the discrete solution to be computed in a time marching fashion. See Figure 4.

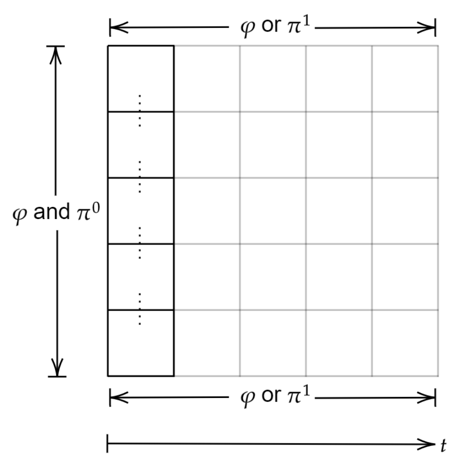

FIGURE 4. Coupling of the discrete forward Hamilton's equations in the same time slice for evolutionary Hamiltonian PDEs; dashed lines along interior edges denote field and normal momenta continuity.

Discrete Noether's Theorem. In the continuum theory, we saw that for a vertical group action on the restricted dual jet bundle which leaves the action invariant, there is an associated Noether conservation law (1.10) for solutions of Hamilton's equations.

In the discrete setting, suppose there is a differentiable and vertical G action on the discrete restricted dual jet bundle $\{t_i, x_j\} \times Q \times (Q^*)^2$ (relative to $\square \in \mathcal{T}(X)$) which leaves invariant the generalized discrete Lagrangian

$$\begin{aligned} R_d^\square(\varphi_{A(\square)}, \varphi_{B(\square)}, \pi_{B(\square)}) &= \sum_{B(\square)} \pi_{B(\square)}\varphi_{B(\square)} - H_d^+(\varphi_{A(\square)}, \pi_{B(\square)}) \\ &= \sum_{i=1}^{s} \Delta t\ b_i \pi^1_{[i]1}\varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x \tilde{b}_\alpha p^0_{1[\alpha]}\varphi_{1[\alpha]} - H_d^+(\{\varphi_{[i]0}, \varphi_{0[\alpha]}, \pi^1_{[i]1}, \pi^0_{1[\alpha]}\}_{i,\alpha}). \end{aligned}$$

Proposition 2.4. *If the generalized discrete Lagrangian is invariant under a differentiable and vertical G action on the discrete restricted dual jet bundle, then a solution of the discrete forward Hamilton's equations (2.3a)-(2.3d) admits a discrete analog of Noether's theorem:*

$$\begin{aligned} &\sum_i \Delta t\ b_i \pi^1_{[i]1} i_{\tilde{\xi}} d\varphi_{[i]1} + \sum_\alpha \Delta x\ \tilde{b}_\alpha \pi^0_{1[\alpha]} i_{\tilde{\xi}} d\varphi_{1[\alpha]} \\ &\qquad - \sum_i \Delta t\ b_i \pi^1_{[i]0} i_{\tilde{\xi}} d\varphi_{[i]0} - \sum_\alpha \Delta x\ \tilde{b}_\alpha \pi^0_{0[\alpha]} i_{\tilde{\xi}} d\varphi_{0[\alpha]} = 0, \end{aligned} \tag{2.5}$$

where $\tilde{\xi}$ is the infinitesimal generator associated with $\xi \in \mathfrak{g}$.

Proof. For brevity, we will omit the arguments of $R_d^\square$ and H_d^+ (refer to the definition of $R_d^\square$ above). Since the generalized discrete Lagrangian is invariant under the G action, that means that the directional derivative in the direction of the infinitesimal generator vanishes,

$$\begin{aligned} 0 &= dR_d^\square \cdot \tilde{\xi} \\ &= \sum_i \Delta t\ b_i i_{\tilde{\xi}} d(\pi^1_{[i]1}\varphi_{[i]1}) + \sum_\alpha \Delta x\ \tilde{b}_\alpha i_{\tilde{\xi}} d(\pi^0_{1[\alpha]}\varphi_{1[\alpha]}) \\ &\quad - \sum_i \Big(D_{1,i} H_d^+ i_{\tilde{\xi}} d\varphi_{[i]0} + D_{3,i} H_d^+ i_{\tilde{\xi}} d\pi^1_{[i]1} \Big) - \sum_\alpha \Big(D_{2,\alpha} H_d^+ i_{\tilde{\xi}} d\varphi_{0[\alpha]} + D_{4,\alpha} H_d^+ i_{\tilde{\xi}} d\pi^0_{1[\alpha]} \Big) \\ &= \sum_i \Delta t\ b_i (\cancelto{(1)}{i_{\tilde{\xi}} d\pi^1_{[i]1}\varphi_{[i]1}} + \pi^1_{[i]1} i_{\tilde{\xi}} d\varphi_{[i]1}) + \sum_\alpha \Delta x\ \tilde{b}_\alpha (\cancelto{(2)}{i_{\tilde{\xi}} d\pi^0_{1[\alpha]}\varphi_{1[\alpha]}} + \pi^0_{1[\alpha]} i_{\tilde{\xi}} d\varphi_{1[\alpha]}) \\ &\quad - \sum_i \Delta t\ b_i \Big(\pi^1_{[i]0} i_{\tilde{\xi}} d\varphi_{[i]0} + \cancelto{(1)}{\varphi_{[i]1} i_{\tilde{\xi}} d\pi^1_{[i]1}} \Big) - \sum_\alpha \Delta x\ \tilde{b}_\alpha \Big(\pi^0_{0[\alpha]} i_{\tilde{\xi}} d\varphi_{0[\alpha]} + \cancelto{(2)}{\varphi_{1[\alpha]} i_{\tilde{\xi}} d\pi^0_{1[\alpha]}} \Big). \end{aligned}$$

$\square$

Remark 2.3. *Note that the above looks like quadrature applied to the continuous Noether's theorem,*

$$\int_{\partial\square} p^\mu (i_{\tilde{\xi}} d\phi) d^n x_\mu = 0$$

(with the caveat that, in the continuum case, G acts on the restricted dual jet bundle, whereas in the discrete case, G acts on the discrete restricted dual jet bundle). One can obtain such a G-invariant R_d via G-equivariant interpolation (see Leok and Zhang [24] and Leok [22]), in which case, the discrete Noether theorem is precisely quadrature applied to Noether's theorem.

Remark 2.4. *Another way to interpret this discrete Noether's theorem is to view the map determined by the discrete forward Hamilton's equations, $(\varphi_{A(\square)}, \pi_{B(\square)}) \mapsto (\varphi_{B(\square)}, \pi_{A(\square)})$, as implicitly defining a forward map $F_{H_d^+} : (\varphi_{A(\square)}, \pi_{A(\square)}) \mapsto (\varphi_{B(\square)}, \pi_{B(\square)})$. For some subset S of $\partial\square$, define the* *discrete (Hamiltonian) Cartan form (at a solution of the discrete forward Hamilton's equations)*

$$\Theta_d^S = \sum_{(t_k,x_l)\in S} \beta_{kl}\pi^n_{kl} d\varphi_{kl}, \tag{2.6}$$

where π^n denotes the normal component of the momenta and β^{kl} denotes the quadrature weight at $(t_k, x_l) \in S$ (which equals $\Delta t\ b_i$ for the i^{th} node of S along fixed x and equals $\Delta x\ \tilde{b}_\alpha$ for the α^{th} node of S along fixed t). Such a discrete Cartan form involving summing over nodes corresponding to boundary variations was introduced by Marsden et al. [28] in the Lagrangian framework; in the discrete Hamiltonian setting which we constructed, (2.6) is the appropriate definition since $\Theta_d^{\partial\square}$ precisely encodes such discrete boundary variations.

Then, the discrete Noether theorem (2.5) can be expressed as

$$F^*_{H_d^+}(\Theta_d^{B(\square)})\cdot\tilde{\xi} = \Theta_d^{A(\square)}\cdot\tilde{\xi}.$$

Note also that the discrete multisymplectic form formula (2.4) can be expressed as

$$d\Theta_d^{\partial\square}(\cdot,\cdot) = 0,$$

when evaluated on discrete first variations.

2.2. **Galerkin Hamiltonian Variational Integrators.** The missing ingredient in our construction of a variational integrator is the discrete approximation of the action over $\square \in \mathcal{T}(X)$, $S_d^\square[\phi, p]$. We will extend the construction of Galerkin Hamiltonian variational integrators, introduced in Leok and Zhang [24] for Hamiltonian ODEs, to the case of Hamiltonian PDEs.

Remark 2.5. *To be definitive, we will assume that the space(time) X has the Euclidean metric. The discussion below is equally valid for the Minkowski metric, except one has to include the appropriate minus signs throughout.*

Consider for simplicity $[0,\Delta t]\times[0,\Delta x] = \square \in \mathcal{T}(X)$. Fix quadrature rules in the temporal direction (weights b_i and nodes c_i, $i = 1,\dots,s$) and spatial direction (weights $\tilde{b}_\alpha$ and nodes $\tilde{c}_\alpha$, $\alpha = 1,\dots,\sigma$) as before. Note the action $S[\phi,p] = \int (p^\mu\partial_\mu\phi - H(\phi,p^0,p^1))d^2x$ involves the fields ϕ, their derivatives $\partial_\mu\phi$, and the multimomenta p^μ ($\mu = 0,1$). For the field and their derivatives, we could either approximate the field using a finite-dimensional subspace and subsequently take derivatives; or conversely, approximate the derivatives and subsequently integrate to obtain the values of the field. We will take the latter approach (we will extremize over the internal stages at the end, so the two approaches are equivalent). Introduce basis functions $\{\chi_i(\tau)\}_{i=1}^s$, $\tau\in[0,1]$, for an s-dimensional function space and similarly $\{\tilde{\chi}_\alpha(\tau)\}_{\alpha=1}^\sigma$ for a σ-dimensional function space. We will use the tensor product basis $\{\chi_i(\tau\Delta t)\tilde{\chi}_\alpha(\rho\Delta x)\}_{i,\alpha}$ to discretize the derivatives of the field. Approximate the derivatives as

$$\partial_t\phi_d(\tau\Delta t,\rho\Delta x) = \sum_{i,\alpha} V^{i\alpha}\chi_i(\tau)\tilde{\chi}_\alpha(\rho), \tag{2.7a}$$

$$\partial_x\phi_d(\tau\Delta t,\rho\Delta x) = \sum_{i,\alpha} W^{i\alpha}\chi_i(\tau)\tilde{\chi}_\alpha(\rho). \tag{2.7b}$$

We can integrate in time or space to determine the field values. In particular, the internal stages are given by the field values at the nodes $(c_i\Delta t, \tilde{c}_\alpha\Delta x)$:

$$\Phi_{i\alpha} \equiv \phi(c_i\Delta t,\tilde{c}_\alpha\Delta x) = \phi(0,\tilde{c}_\alpha\Delta x) + \Delta t\sum_{j,\beta} V^{j\beta}\int_0^{c_i}\chi_j(s)ds\ \tilde{\chi}_\beta(\tilde{c}_\alpha) = \varphi_{0[\alpha]} + \Delta t\sum_{j,\beta} A_{i\alpha,j\beta}V^{j\beta},$$

$$\Phi_{i\alpha} \equiv \phi(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \phi(c_i\Delta t, 0) + \Delta x \sum_{j,\beta} W^{j\beta}\chi_j(c_i)\int_0^{c_\alpha} \tilde{\chi}_\beta(s)ds = \varphi_{[i]0} + \Delta x \sum_{j,\beta} \tilde{A}_{i\alpha,j\beta}W^{j\beta},$$

where $A_{i\alpha,j\beta} = \int_0^{c_i} \chi_j(s)ds\ \tilde{\chi}_\beta(\tilde{c}_\alpha)$ and $\tilde{A}_{i\alpha,j\beta} = \chi_j(c_i)\int_0^{c_\alpha} \tilde{\chi}_\beta(s)ds$. Note that $\Phi_{i\alpha}$ must of course be single-valued, so we have a relation between the two above equations:

$$\phi_{0[\alpha]} + \Delta t A_{i\alpha,j\beta}V^{j\beta} = \Phi_{i\alpha} = \phi_{[i]0} + \Delta x \tilde{A}_{i\alpha,j\beta}W^{j\beta}. \tag{2.8}$$

We expect such a relation since extremizing over $\Phi_{i\alpha}$ is equivalent to extremizing over $V_{i\alpha}$ or $W_{i\alpha}$ (but not both; however, we will relax this assumption in the subsequent discussion).

Integrating to 1 gives the unknown field boundary values,

$$\varphi_{1[\alpha]} \equiv \phi(\Delta t, \tilde{c}_\alpha\Delta x) = \phi(0, \tilde{c}_\alpha\Delta x) + \Delta t \sum_{j,\beta} V^{j\beta}\int_0^1 \chi_j(s)ds\ \tilde{\chi}_\beta(\tilde{c}_\alpha) = \varphi_{0[\alpha]} + \Delta t\sum_{j,\beta} B_{\alpha,j\beta}V^{j\beta},$$

$$\varphi_{[i]1} \equiv \phi(c_i\Delta t, \Delta x) = \phi(c_i\Delta t, 0) + \Delta x \sum_{j,\beta} W^{j\beta}\chi_j(c_i)\int_0^1 \tilde{\chi}_\beta(s)ds = \varphi_{[i]0} + \Delta x\sum_{j,\beta} \tilde{B}_{i,j\beta}W^{j\beta},$$

where $B_{\alpha,j\beta} = \int_0^1 \chi_j(s)ds\ \tilde{\chi}_\beta(\tilde{c}_\alpha)$ and $\tilde{B}_{i,j\beta} = \chi_j(c_i)\int_0^1 \tilde{\chi}_\beta(s)ds$.

We define the internal stages for the momenta $P^0_{i\alpha} = p^0(c_i\Delta t, \tilde{c}_\alpha\Delta x), P^1_{i\alpha} = p^1(c_i\Delta t, \tilde{c}_\alpha\Delta x)$. Unlike the field internal stage expansions, one does not need to introduce an approximating function space for the momenta internal stages, since the action only involves derivatives of the field and not the momenta. At this point, we could work directly with these internal stages; however, we will expand the momenta similarly to the fields,

$$P^0_{i\alpha} = \pi^0_{1[\alpha]} - \Delta t\sum_{j,\beta} A'_{i\alpha,j\beta}X^{j\beta},$$

$$P^1_{i\alpha} = \pi^1_{[i]1} - \Delta x\sum_{j,\beta} \tilde{A}'_{i\alpha,j\beta}Y^{j\beta},$$

where $A'_{i\alpha,j\beta}$ and $\tilde{A}'_{i\alpha,j\beta}$ are arbitrary expansion coefficients and $X^{j\beta}, Y^{j\beta}$ are internal variables representing $\partial_0 p^0$ and $\partial_1 p^1$ respectively. The unknown momenta boundary values are similarly defined as

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t\sum_{j,\beta} B'_{\alpha,j\beta}X^{j\beta},$$

$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x\sum_{j,\beta} \tilde{B}'_{i,j\beta}Y^{j\beta},$$

where $B'_{\alpha,j\beta}$ and $\tilde{B}'_{i,j\beta}$ are again arbitrary expansion coefficients. We will see later that the expansion coefficients will have to satisfy symplecticity conditions in order for the method to be well-defined.

We then approximate the action integral $S[\phi, p] = \int(p^\mu\partial_\mu\phi - H(\phi, p^0, p^1))d^2x$ using quadrature and the above internal stages

$$S^\square_d[\Phi_{i\alpha}, P_{i\alpha}] = \Delta t\Delta x\sum_{i,\alpha} b_i\tilde{b}_\alpha\Big(P^0_{i\alpha}\partial_t\phi_d(c_i\Delta t, \tilde{c}_\alpha\Delta x) + P^1_{i\alpha}\partial_x\phi_d(c_i\Delta t, \tilde{c}_\alpha\Delta x) - H(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})\Big).$$

The discrete boundary Hamiltonian is obtained by extremizing over the internal stages Φ, P^0, P^1, which are defined in terms of V, X, Y. Since we have already enforced the boundary conditions in the above field and momenta expansions, we can construct the discrete boundary Hamiltonian by extremizing over $V^{i\alpha}$, $X^{i\alpha}$, $Y^{i\alpha}$ (for every $i = 1, \dots, s$ and $\alpha = 1, \dots, \sigma$),

$$H_d^+(\{\varphi_{[i]0}, \varphi_{0[\alpha]}, \pi^1_{[i]1}, \pi^0_{1[\alpha]}\}_{i,\alpha}) = \operatorname*{ext}_{V^{i\alpha}, X^{i\alpha}, Y^{i\alpha}} \underbrace{\Big(\sum_{i=1}^{s} \Delta t\ b_i \pi^1_{[i]1} \varphi_{[i]1} + \sum_{\alpha=1}^{\sigma} \Delta x\ \tilde{b}_\alpha \pi^0_{1[\alpha]} \varphi_{1[\alpha]} - S_d^\square[\Phi_{i\alpha}, P_{i\alpha}] \Big)}_{\equiv K(\{\varphi_A, \pi_B, V^{i\alpha}, X^{i\alpha}, Y^{i\alpha}\})}.$$

H_d^+ is then given by extremizing $K(\{\varphi_A, \pi_B, V^{i\alpha}, X^{i\alpha}, Y^{i\alpha}\})$ with respect to $V^{i\alpha}, X^{i\alpha}$, and $Y^{i\alpha}$ (where again we denote $\varphi_A = \{\varphi_{[i]0}, \varphi_{0[\alpha]}\}$ and $\pi_B = \{\pi^1_{[i]1}, \pi^0_{1[\alpha]}\}$). Expanding K, we have

$$\begin{aligned}
&K(\{\varphi_A, \pi_B, V^{i\alpha}, X^{i\alpha}, Y^{i\alpha}\}) \\
&\quad = \Delta t \sum_i b_i \pi^1_{[i]1} (\varphi_{[i]0} + \Delta x \sum_{j,\beta} \tilde{B}_{i,j\beta} W^{j\beta}) + \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]} (\varphi_{0[\alpha]} + \Delta t \sum_{j,\beta} B_{\alpha,j\beta} V^{j\beta}) \\
&\qquad - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^0_{1[\alpha]} - \Delta t \sum_{k,\gamma} A'_{i\alpha,k\gamma} X^{k\gamma} \Big) \sum_{j,\beta} V^{j\beta} \chi_j(c_i) \tilde{\chi}_\alpha(\tilde{c}_\alpha) \\
&\qquad - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^1_{[i]1} - \Delta x \sum_{k,\gamma} \tilde{A}'_{i\alpha,k\gamma} Y^{k\gamma} \Big) \sum_{j,\beta} W^{j\beta} \chi_j(c_i) \tilde{\chi}_\alpha(\tilde{c}_\alpha) \\
&\qquad + \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).
\end{aligned}$$

The stationarity conditions $\partial K/\partial V^{i\alpha} = 0$, $\partial K/\partial X^{i\alpha} = 0$, $\partial K/\partial Y^{i\alpha} = 0$, combined with the discrete forward Hamilton's equations (2.3a)-(2.3d) define our multisymplectic variational integrator.

Supposing that one solves the stationarity conditions for $V^{i\alpha}$, $X^{i\alpha}$, $Y^{i\alpha}$ in terms of φ_A and π_B, this gives $H_d^+(\{\varphi_A, \pi_B\}) = K(\{\varphi_A, \pi_B, V^{i\alpha}(\varphi_A, \pi_B), X^{i\alpha}(\varphi_A, \pi_B), Y^{i\alpha}(\varphi_A, \pi_B)\})$. The right hand side of the discrete forward Hamilton's equations, (2.3a)-(2.3d), can then be computed in terms of K via

$$\begin{aligned}
\frac{\partial}{\partial \varphi_{[i]0}} H_d^+(\{\varphi_A, \pi_B\}) &= \frac{\partial}{\partial \varphi_{[i]0}} K(\{\varphi_A, \pi_B, V^{i\alpha}(\varphi_A, \pi_B), X^{i\alpha}(\varphi_A, \pi_B), Y^{i\alpha}(\varphi_A, \pi_B)\}) \\
&= \frac{\partial}{\partial \varphi_{[i]0}} K + \sum_{j,\alpha} \Big(\cancel{\frac{\partial K}{\partial V^{j\alpha}}} \frac{\partial V^{j\alpha}}{\partial \varphi_{[i]0}} + \cancel{\frac{\partial K}{\partial X^{j\alpha}}} \frac{\partial X^{j\alpha}}{\partial \varphi_{[i]0}} + \cancel{\frac{\partial K}{\partial Y^{j\alpha}}} \frac{\partial Y^{j\alpha}}{\partial \varphi_{[i]0}} \Big) \\
&= \frac{\partial}{\partial \varphi_{[i]0}} K,
\end{aligned}$$

and similarly for the other specified boundary values. Hence, the derivatives of H_d^+ with respect to φ_A, π_B can be computed using only the explicit dependence of K on φ_A, π_B.

2.3. **Multisymplectic Partitioned Runge–Kutta Method.** Let us suppose that instead of the basis $\{\chi_i\}, \{\tilde{\chi}_\alpha\}$, we choose basis functions $\{\psi_i\}$, $\{\tilde{\psi}_\alpha\}$ that have the interpolating property $\psi_i(c_j) = \delta_{ij}$, $\tilde{\psi}_\alpha(\tilde{c}_\beta) = \delta_{\alpha\beta}$. Note that one can always transform the previous set of basis functions to a set of basis functions with this property, assuming that the original choice of basis functions $\chi_i, \tilde{\chi}_\alpha$ have the property that the matrices with entries $M_{ij} = \chi_i(c_j)$, $\tilde{M}_{\alpha\beta} = \tilde{\chi}_\alpha(\tilde{c}_\beta)$ are invertible. If they are not, then the expansion of the derivatives, equations (2.7a)-(2.7b), does not depend independently on all of the $V^{i\alpha}$, $W^{i\alpha}$ and hence one needs to reduce the number of independent variables; to avoid this, ensure that the matrices with entries $\chi_i(c_j)$ and $\tilde{\chi}_\alpha(\tilde{c}_\beta)$ are invertible. Letting $\chi(\cdot) = (\chi_1(\cdot), \dots, \chi_s(\cdot))^T$ and $\tilde{\chi}(\cdot) = (\tilde{\chi}_1(\cdot), \dots, \tilde{\chi}_\sigma(\cdot))^T$ (and similarly define ψ, $\tilde{\psi}$), a set of basis functions with the interpolating property can be constructed by $\psi = M^{-1}\chi$, $\tilde{\psi} = \tilde{M}^{-1}\tilde{\chi}$. In particular, the $\{\psi_i\}$, $\{\tilde{\psi}_\alpha\}$ span the same function spaces as the $\{\chi_i\}$, $\{\tilde{\chi}_\alpha\}$ respectively, so there is no loss of generality.

With this assumption, we approximate the derivatives of the fields as

$$\partial_t \phi_d(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \sum_{j,\beta} V^{j\beta}\psi_j(c_i)\tilde{\psi}_\beta(\tilde{c}_\alpha) = V^{i\alpha},$$
$$\partial_x \phi_d(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \sum_{j,\beta} W^{j\beta}\psi_j(c_i)\tilde{\psi}_\beta(\tilde{c}_\alpha) = W^{i\alpha}.$$

Integrating gives the internal stages and the unknown boundary values,

$$\begin{aligned}
\Phi_{i\alpha} &= \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha},\\
\Phi_{i\alpha} &= \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta}\\
\varphi_{1[\alpha]} &= \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha},\\
\varphi_{[i]1} &= \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta},
\end{aligned}$$

where $a_{ij} = \int_0^{c_i}\psi_j(s)ds$, $\tilde{a}_{\alpha\beta} = \int_0^{\tilde{c}_\alpha}\tilde{\psi}_\beta(s)ds$ and the quadrature weights $b_i = \int_0^1 \psi_i(s)ds$, $\tilde{b}_\alpha = \int_0^1 \tilde{\psi}_\alpha(s)ds$ are chosen so that quadrature is exact on the span of the basis functions. As before, expand the momenta using a different set of coefficients.

$$\begin{aligned}
X^{i\alpha} &= \partial_t p_d^0(c_i\Delta t, \tilde{c}_\alpha\Delta x),\\
Y^{i\alpha} &= \partial_x p_d^1(c_i\Delta t, \tilde{c}_\alpha\Delta x),\\
P^0_{i\alpha} &= \pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha},\\
P^1_{i\alpha} &= \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta},\\
\pi^0_{0[\alpha]} &= \pi^0_{1[\alpha]} - \Delta t \sum_j b'_j X^{j\alpha},\\
\pi^1_{[i]0} &= \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{b}'_\beta Y^{i\beta}.
\end{aligned}$$

We impose that $b'_j > 0$, $\tilde{b}'_\beta > 0$ and that $\sum_j b'_j = 1$, $\sum_\beta \tilde{b}'_\beta = 1$ for the approximation to be consistent. We will later derive a condition on the coefficients a'_{ij}, $\tilde{a}'_{\alpha\beta}$, b'_i, $\tilde{b}'_\alpha$ in order for the method to be well-defined. For now, we proceed formally.

With these, K can be expressed as

$$\begin{aligned}
&K(\{\varphi_A, \pi_B, V^{i\alpha}, X^{i\alpha}, Y^{i\alpha}\})\\
&\quad = \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]}(\varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}) + \Delta t \sum_i b_i \pi^1_{[i]1}(\varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta})\\
&\qquad - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha}\Big) V^{i\alpha}\\
&\qquad - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta}\Big) W^{i\alpha}
\end{aligned}$$

$$+ \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

Now, we compute the stationarity conditions. First, note that V and W are not independent, since they are related by

$$\varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha} = \Phi_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta};$$

then, taking the derivative with respect to $V^{j\beta}$,

$$\Delta t a_{ij} \delta_{\alpha\beta} = \Delta x \sum_\gamma \tilde{a}_{\alpha\gamma} \frac{\partial W^{i\gamma}}{\partial V^{j\beta}}.$$

Let us assume that the Runge–Kutta matrices (a_{ij}) and $(\tilde{a}_{\alpha\gamma})$ are invertible (however, in the subsequent section, we will show how to derive the stationarity conditions without this assumption using independent internal stages). Then, the above relation can be inverted to give

$$\frac{\partial W^{i\sigma}}{\partial V^{j\beta}} = \frac{\Delta t}{\Delta x} a_{ij} (\tilde{a}^{-1})_{\sigma\beta}.$$

Extremizing K with respect to $X^{j\alpha}$,

$$0 = \frac{\partial K}{\partial X^{j\alpha}} = \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\alpha a'_{ij} V^{i\alpha} - \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\alpha a'_{ij} \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

Dividing by $\Delta t^2 \Delta x \tilde{b}_\alpha$ gives

$$\sum_i b_i a'_{ij} \Big(V^{i\alpha} - \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \Big) = 0.$$

Similarly, extremizing K with respect to $Y^{j\alpha}$ gives

$$\sum_\beta \tilde{b}_\beta \tilde{a}'_{\beta\alpha} \Big(W^{j\beta} - \frac{\partial H}{\partial p^1}(\Phi_{j\beta}, P^0_{j\beta}, P^1_{j\beta}) \Big) = 0.$$

These are respectively the internal stage approximations to the De Donder–Weyl equations $\partial_t \phi = \partial H/\partial p^0$ and $\partial_x \phi = \partial H / \partial p^1$.

Extremizing K with respect to $V^{j\beta}$,

$$0 = \frac{\partial K}{\partial V^{j\beta}} = \Delta t \Delta x b_j \tilde{b}_\beta \pi^0_{1[\beta]} + \Delta t \Delta x \sum_{i,\sigma} b_i \tilde{b}_\sigma \pi^1_{[i]1} \frac{\Delta t}{\Delta x} a_{ij} (\tilde{a}^{-1})_{\sigma\beta} - \Delta t \Delta x b_j \tilde{b}_\beta P^0_{j\beta}$$
$$- \Delta t \Delta x \sum_{i,\sigma} b_i \tilde{b}_\sigma P^1_{i\sigma} \frac{\Delta t}{\Delta x} a_{ij} (\tilde{a}^{-1})_{\sigma\beta} + \Delta t \Delta x \sum_i b_i \tilde{b}_\beta \Delta t a_{ij} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Dividing by $\Delta t^2 \Delta x$ and grouping gives

$$b_j \tilde{b}_\beta \frac{\pi^0_{1[\beta]} - P^0_{j\beta}}{\Delta t} + \sum_{i,\sigma} b_i \tilde{b}_\sigma a_{ij} (\tilde{a}^{-1})_{\sigma\beta} \frac{\pi^1_{[i]1} - P^1_{i\sigma}}{\Delta x} = - \sum_i b_i \tilde{b}_\beta a_{ij} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Substitute $\frac{\pi^0_{1[\beta]} - P^0_{j\beta}}{\Delta t} = \sum_k a'_{jk} X^{k\beta}$ and $\frac{\pi^1_{[i]1} - P^1_{i\sigma}}{\Delta x} = \sum_\gamma \tilde{a}'_{\sigma\gamma} Y^{i\gamma}$,

$$\sum_k b_j \tilde{b}_\beta a'_{jk} X^{k\beta} + \sum_{i,\sigma,\gamma} b_i \tilde{b}_\sigma a_{ij} (\tilde{a}^{-1})_{\sigma\beta} \tilde{a}'_{\sigma\gamma} Y^{i\gamma} = - \sum_i b_i \tilde{b}_\beta a_{ij} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

To symmetrize the above equations, multiply by $\tilde{a}_{\beta\delta}$ and sum over β, which yields

$$\sum_{k,\beta} b_j \tilde{b}_\beta a'_{jk} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}_\delta a_{ij} \tilde{a}'_{\delta\gamma} Y^{i\gamma} = -\sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

This is the internal stage approximation to the remaining De Donder–Weyl equation $\partial_t p^0 + \partial_x p^1 = -\partial H/\partial\phi$. Note that the above form of the stationarity condition does not involve a^{-1} or $\tilde{a}^{-1}$, so it is plausible that one can derive these equations without assuming the invertibility of the Runge–Kutta matrices; later, we will show that this is the case using independent internal stages.

Now, we compute the discrete forward Hamilton's equations. We have

$$\begin{aligned}
\varphi_{1[\alpha]} &= \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial H_d^+}{\partial \pi^0_{1[\alpha]}} \\
&= \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \pi^0_{1[\alpha]}} \\
&= \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha} - \Delta t \sum_j b_j V^{j\alpha} + \Delta t \sum_j b_j \frac{\partial H}{\partial p^0}(\Phi_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) \\
&= \varphi_{0[\alpha]} + \Delta t \sum_j b_j \frac{\partial H}{\partial p^0}(\Phi_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}).
\end{aligned}$$

Similarly,

$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta \frac{\partial H}{\partial p^1}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Computing the discrete forward Hamilton's equations for the momenta gives

$$\begin{aligned}
\pi^0_{0[\alpha]} &= \pi^0_{1[\alpha]} + \frac{\Delta t}{\tilde{b}_\alpha} \sum_{i,\beta} b_i \tilde{b}_\beta \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) \frac{\partial \Phi_{i\beta}}{\partial \varphi_{0[\alpha]}}, \\
\pi^1_{[i]0} &= \pi^1_{[i]1} + \frac{\Delta x}{b_i} \sum_{j,\alpha} b_j \tilde{b}_\alpha \frac{\partial H}{\partial \phi}(\Phi_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) \frac{\partial \Phi_{j\alpha}}{\partial \varphi_{[i]0}}.
\end{aligned}$$

We will postpone the discussion of the discrete forward Hamilton's equations until after discussing independent internal stages, which will give a more explicit characterization of these equations.

To summarize, our method is given by

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha}, \tag{2.9a}$$

$$P^0_{i\alpha} = \pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha}, \tag{2.9b}$$

$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}, \tag{2.9c}$$

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_j b'_j X^{j\alpha}, \tag{2.9d}$$

$$\Phi_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta} \tag{2.9e}$$

$$P^1_{i\alpha} = \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta}, \tag{2.9f}$$

$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}, \tag{2.9g}$$

$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{b}'_\beta Y^{i\beta}. \tag{2.9h}$$

$$\sum_i b_i a'_{ij} \Big(V^{i\alpha} - \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \Big) = 0, \tag{2.9i}$$

$$\sum_\beta \tilde{b}_\beta \tilde{a}'_{\beta\alpha} \Big(W^{j\beta} - \frac{\partial H}{\partial p^1}(\Phi_{j\beta}, P^0_{j\beta}, P^1_{j\beta}) \Big) = 0, \tag{2.9j}$$

$$\sum_{k,\beta} b_j \tilde{b}_\beta a'_{jk} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}_\delta a_{ij} \tilde{a}'_{\delta\gamma} Y^{i\gamma} = - \sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi_{i\beta}, P^0_{i\beta}, P^1_{i\beta}). \tag{2.9k}$$

Independent Internal Stages. We now reformulate the above construction using independent internal stages and derive explicit conditions on the coefficients for the momenta expansion for the method to be well-defined. Recall that in the above construction, we enforced the condition that the internal stages $\Phi_{i\alpha}$ produced by both $V^{i\alpha}$ and $W^{i\alpha}$ had to be the same; we now relax this assumption and let the internal stages be independent, but subsequently enforce that they are the same by using Lagrange multipliers. Compared to the previous formulation, the use of independent internal stages has the advantage that the discrete forward Hamilton's equations can be written explicitly. Furthermore, the generalization to higher spacetime dimensions is straight-forward as opposed to the previous formulation, which would involve inverting the condition that the internal stages obtained from the various spacetime derivative approximations, $\partial_\mu \phi_d$, are consistent.

Hence, we define independent internal stages corresponding to integration in each spacetime direction,

$$\Phi_{i\alpha} \equiv \phi(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \phi(0, \tilde{c}_\alpha \Delta x) + \Delta t \sum_{j,\beta} V^{j\beta} \int_0^{c_i} \psi_j(s) ds \; \tilde{\psi}_\beta(\tilde{c}_\alpha) = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha},$$
$$\tilde{\Phi}_{i\alpha} \equiv \phi(c_i\Delta t, \tilde{c}_\alpha \Delta x) = \phi(c_i\Delta t, 0) + \Delta x \sum_{j,\beta} W^{j\beta} \psi_j(c_i) \int_0^{\tilde{c}_\alpha} \tilde{\psi}_\beta(s) ds = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta}.$$

The expansion of the other quantities are the same as the previous discussion.

We will evaluate the Hamiltonian at the weighted combination $\Phi^\theta_{i\alpha} \equiv \theta\Phi_{i\alpha} + (1-\theta)\tilde{\Phi}_{i\alpha}$ for some arbitrary parameter $\theta \in \mathbb{R}$ and subsequently enforce that the two sets of internal stages are the same through a Lagrange multiplier term $\sum_{i,\alpha} \lambda_{i\alpha}(\Phi_{i\alpha} - \tilde{\Phi}_{i\alpha})$. Thus, after enforcing the stationarity conditions, $\Phi^\theta_{i\alpha} = \Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$. In this formulation, K is

$$\begin{aligned} K(\{\varphi_A, \pi_B, V^{i\alpha}, W^{i\alpha}, X^{i\alpha}, Y^{i\alpha}, \lambda_{i\alpha}\}) = \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]} (\varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}) \\ + \Delta t \sum_i b_i \pi^1_{[i]1} (\varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}) \\ - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^0_{1[\alpha]} - \Delta t \sum_j a'_{ij} X^{j\alpha} \Big) V^{i\alpha} \end{aligned}$$

$$- \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \Big(\pi^1_{[i]1} - \Delta x \sum_\beta \tilde{a}'_{\alpha\beta} Y^{i\beta} \Big) W^{i\alpha}$$
$$+ \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \sum_{i,\alpha} \lambda_{i\alpha}(\Phi_{i\alpha} - \tilde{\Phi}_{i\alpha});$$

where now both $\{V^{i\alpha}\}$ and $\{W^{i\alpha}\}$ are independent. The discrete boundary Hamiltonian H_d^+ is given by extremizing K with respect to all of the internal variables, $\{V^{i\alpha}, W^{i\alpha}, X^{i\alpha}, Y^{i\alpha}, \lambda_{i\alpha}\}$.

Extremizing K with respect to $X^{j\alpha}$ and $Y^{j\alpha}$ gives the same stationarity conditions as the previous case of equal internal stages, since the momenta expansions were unchanged, except with H evaluated at $\Phi^\theta_{i\alpha}$. Namely,

$$\sum_i b_i a'_{ij} \Big(V^{i\alpha} - \frac{\partial H}{\partial p^0}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \Big) = 0, \tag{2.10a}$$

$$\sum_\beta \tilde{b}_\beta \tilde{a}'_{\beta\alpha} \Big(W^{j\beta} - \frac{\partial H}{\partial p^1}(\Phi^\theta_{j\beta}, P^0_{j\beta}, P^1_{j\beta}) \Big) = 0. \tag{2.10b}$$

Extremizing K with respect to $V^{j\beta}$,

$$0 = \frac{\partial K}{\partial V^{j\beta}} = \Delta t \Delta x b_j \tilde{b}_\beta \pi^0_{1[\beta]} - \Delta t \Delta x b_j \tilde{b}_\beta P^0_{j\beta} + \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \Delta t \sum_i \lambda_{i\beta} a_{ij}$$
$$= \Delta t^2 \Delta x b_j \tilde{b}_\beta \sum_k a'_{jk} X^{k\beta} + \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \Delta t \sum_i \lambda_{i\beta} a_{ij}.$$

Dividing by $\Delta t^2 \Delta x$,

$$\sum_k b_j \tilde{b}_\beta a'_{jk} X^{k\beta} + \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \frac{1}{\Delta t \Delta x} \sum_i \lambda_{i\beta} a_{ij} = 0. \tag{2.11}$$

Similarly, extremizing K with respect to $W^{j\beta}$ (and dividing by $\Delta t \Delta x^2$) gives

$$\sum_\alpha b_j \tilde{b}_\beta \tilde{a}'_{\beta\alpha} Y^{j\alpha} + \sum_\alpha b_j \tilde{b}_\alpha \tilde{a}_{\alpha\beta} (1-\theta) \frac{\partial H}{\partial \phi}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) - \frac{1}{\Delta t \Delta x} \sum_\alpha \lambda_{j\alpha} \tilde{a}_{\alpha\beta} = 0. \tag{2.12}$$

Let us combine these two stationarity conditions to eliminate θ and the Lagrange multiplier terms. Multiply equation (2.11) by $\tilde{a}_{\beta\delta}$ and sum over β; multiply equation (2.12) by a_{ji} and sum over j. Subsequently, add the two resulting equations. This gives

$$\sum_{k,\beta} b_j \tilde{b}_\beta a'_{jk} \tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}_\delta a_{ij} \tilde{a}'_{\delta\gamma} Y^{i\gamma} = - \sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}). \tag{2.13}$$

Finally, extremizing K with respect to $\lambda_{i\alpha}$ enforces that the independent internal stages are the same, $0 = \partial K / \partial \lambda_{i\alpha} = \Phi_{i\alpha} - \tilde{\Phi}_{i\alpha}$, and hence $\Phi^\theta_{i\alpha} = \Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$. We have rederived the stationarity conditions that we saw in the case of equal internal stages, without the assumption of invertibility of the Runge–Kutta matrices, (a_{ij}), $(\tilde{a}_{\alpha\beta})$.

Now, we aim to provide a more explicit characterization of the discrete forward Hamilton's equations. We will assume again that the Runge–Kutta matrices (a_{ij}), $(\tilde{a}_{\alpha\beta})$ are invertible. Computing the discrete forward Hamilton's equations for the field boundary values,

$$\varphi_{1[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial H_d^+}{\partial \pi^0_{1[\alpha]}} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \pi^0_{1[\alpha]}} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j \frac{\partial H}{\partial p^0}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^0_{j\alpha}),$$

$$\varphi_{[i]1} = \frac{1}{b_i \Delta t} \frac{\partial H_d^+}{\partial \pi^1_{[i]1}} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \pi^1_{[i]1}} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Recall that we also have the expansion for the field boundary values

$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha},$$

$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}.$$

We will see shortly that, with a particular condition on the coefficients of the momenta expansion, the discrete forward Hamilton's equations for the field values are consistent with the field expansions, i.e., that $V^{j\alpha} = \frac{\partial H}{\partial p^0}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^0_{j\alpha})$ and similarly $W^{i\beta} = \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta})$.

First, we compute the discrete forward Hamilton's equations for the momenta boundary values,

$$\pi^0_{0[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial H_d^+}{\partial \varphi_{0[\alpha]}} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \varphi_{0[\alpha]}} = \pi^0_{1[\alpha]} + \Delta t \sum_i b_i \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \frac{1}{\tilde{b}_\alpha \Delta x} \sum_i \lambda_{i\alpha},$$

$$\pi^1_{[i]0} = \frac{1}{b_i \Delta t} \frac{\partial H_d^+}{\partial \varphi_{[i]0}} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \varphi_{[i]0}} = \pi^1_{[i]1} + \Delta x \sum_\alpha \tilde{b}_\alpha (1-\theta) \frac{\partial H}{\partial \theta}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) - \frac{1}{b_i \Delta t} \sum_\alpha \lambda_{i\alpha}.$$

For our method to be well-defined, these are required to be consistent with the momenta expansions,

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_j b'_j X^{j\alpha},$$

$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_\beta \tilde{b}'_\beta Y^{i\beta}.$$

To do this, we solve the stationarity conditions (2.11) and (2.12) for the Lagrange multipliers. Multiply equation (2.11) by $(a^{-1})_{jl}$ and sum over j; multiply equation (2.12) by $(\tilde{a}^{-1})_{\beta\gamma}$ and sum over β. This gives

$$\lambda_{l\beta} = -\Delta t \Delta x b_l \tilde{b}_\beta \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{l\beta}, P^0_{l\beta}, P^1_{l\beta}) - \Delta t \Delta x \sum_{j,k} b_j \tilde{b}_\beta a'_{jk} (a^{-1})_{jl} X^{k\beta},$$

$$\lambda_{j\gamma} = \Delta t \Delta x b_j \tilde{b}_\gamma (1-\theta) \frac{\partial H}{\partial \phi}(\Phi^\theta_{j\gamma}, P^0_{j\gamma}, P^1_{j\gamma}) + \Delta t \Delta x \sum_{\alpha,\beta} b_j \tilde{b}_\beta \tilde{a}'_{\beta\alpha} (\tilde{a}^{-1})_{\beta\gamma} Y^{j\alpha}.$$

Plugging these into the respective discrete forward Hamilton's equations for the momenta boundary values, we have

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_{j,k,l} b_j a'_{jk} (a^{-1})_{jl} X^{k\beta} \stackrel{!}{=} \pi^0_{1[\alpha]} - \Delta t \sum_k b'_k X^{k\alpha},$$

$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_{\alpha,\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha} (\tilde{a}^{-1})_{\beta\gamma} Y^{i\alpha} \stackrel{!}{=} \pi^1_{[i]1} - \Delta x \sum_\alpha \tilde{b}'_\alpha Y^{i\alpha}.$$

Proposition 2.5. *The method arising from approximating the internal stages with the partitioned Runge–Kutta expansion is well-defined if and only if the partitioned Runge–Kutta method is symplectic in both space and time, i.e.*

$$\sum_{j,l} b_j a'_{jk} (a^{-1})_{jl} = b'_k,$$

$$\sum_{\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha} (\tilde{a}^{-1})_{\beta\gamma} = \tilde{b}'_\alpha.$$

A sufficient condition is the usual choice of symplectic partitioned Runge–Kutta coefficients,

$$a'_{jk} = \frac{b'_k a_{kj}}{b_j},$$
$$\tilde{a}'_{\beta\alpha} = \frac{\tilde{b}'_\alpha \tilde{a}_{\alpha\beta}}{\tilde{b}_\beta}.$$

(We will see after expressing the momenta internal stages in terms of π_A instead of π_B that these are the usual choice of symplectic partitioned Runge–Kutta coefficients).

Proof. By comparing the momenta expansions to the discrete forward Hamilton's equations for the momenta, we must have

$$\sum_{j,k,l} b_j a'_{jk}(a^{-1})_{jl} X^{k\beta} = \sum_k b'_k X^{k\alpha}, \tag{2.14a}$$

$$\sum_{\alpha,\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha}(\tilde{a}^{-1})_{\beta\gamma} Y^{i\alpha} = \sum_\alpha \tilde{b}'_\alpha Y^{i\alpha}. \tag{2.14b}$$

Since the internal variables $\{X^{i\alpha}, Y^{i\alpha}\}$ are generally arbitrary (depending on the choice of Hamiltonian and the supplied boundary data), the above must hold for arbitrary choices of $\{X^{i\alpha}\}$ and $\{Y^{i\alpha}\}$; hence, we have the necessary and sufficient conditions

$$\sum_{j,l} b_j a'_{jk}(a^{-1})_{jl} = b'_k,$$
$$\sum_{\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha}(\tilde{a}^{-1})_{\beta\gamma} = \tilde{b}'_\alpha.$$

Plugging in the choice (2.14a) and (2.14b) to the left hand sides of the above conditions,

$$\sum_{j,l} b_j a'_{jk}(a^{-1})_{jl} = \sum_{j,l} b'_k a_{kj}(a^{-1})_{jl} = \sum_l b'_k \delta_{kl} = b'_k,$$
$$\sum_{\beta,\gamma} \tilde{b}_\beta \tilde{a}'_{\beta\alpha}(\tilde{a}^{-1})_{\beta\gamma} = \sum_{\beta,\gamma} \tilde{b}'_\alpha \tilde{a}_{\alpha\beta}(\tilde{a}^{-1})_{\beta\gamma} = \sum_\gamma \tilde{b}'_\alpha \delta_{\alpha\gamma} = \tilde{b}'_\alpha;$$

so this choice is sufficient for the method to be well-defined. □

Now, consider the stationarity conditions (2.10a) and (2.10b). Plugging in the choice of coefficients (2.14a) and (2.14b), we have

$$\sum_i b'_j a_{ji}\Big(V^{i\alpha} - \frac{\partial H}{\partial p^0}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})\Big) = 0,$$
$$\sum_\beta \tilde{b}'_\alpha \tilde{a}_{\alpha\beta}\Big(W^{j\beta} - \frac{\partial H}{\partial p^1}(\Phi^\theta_{j\beta}, P^0_{j\beta}, P^1_{j\beta})\Big) = 0.$$

Since (a_{ji}) and $(\tilde{a}_{\alpha\beta})$ are invertible, we have $V^{j\alpha} = \frac{\partial H}{\partial p^0}(\Phi^\theta_{j\alpha}, P^0_{j\alpha}, P^0_{j\alpha})$ and $W^{i\beta} = \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta})$ so that the discrete forward Hamilton's equations for the field boundary values are also consistent with the their expansions. Similarly, plugging this choice of coefficients into the stationarity condition (2.13) gives

$$\sum_{k,\beta} b'_k \tilde{b}_\beta a_{kj}\tilde{a}_{\beta\delta} X^{k\beta} + \sum_{i,\gamma} b_i \tilde{b}'_\gamma a_{ij}\tilde{a}_{\gamma\delta} Y^{i\gamma} = -\sum_{i,\beta} b_i \tilde{b}_\beta a_{ij}\tilde{a}_{\beta\delta}\frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

To invert this relation, we impose $b'_k = b_k, \tilde{b}'_\gamma = \tilde{b}_\gamma$. Note that the matrix with jk entry $b_k a_{kj}$ is invertible since (a_{jk}) is (its transpose is obtained by multiplying the i^{th} row of (a_{ij}) by $b_i \neq 0$, so the rows are still linearly independent) and similarly for the matrix with $\delta\gamma$ entry $\tilde{b}_\gamma \tilde{a}_{\gamma\delta}$. Hence, this stationarity condition can be inverted to give

$$X^{i\alpha} + Y^{i\alpha} = -\frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

Finally, to write our method in the traditional form of a partitioned Runge–Kutta method, we express the internal stages $P^0_{i\alpha}$ and $P^1_{i\alpha}$ in terms of π_A instead of π_B, by plugging equations (2.9d) and (2.9h) into equations (2.9b) and (2.9f) respectively,

$$P^0_{i\alpha} = \pi^0_{0[\alpha]} + \Delta t \sum_j (b_j - a'_{ij}) X^{j\alpha} = \pi^0_{0[\alpha]} + \Delta t \sum_j \underbrace{\frac{b_j b_i - b_j a_{ji}}{b_i}}_{\equiv a^{(2)}_{ij}} X^{j\alpha},$$

$$P^1_{i\alpha} = \pi^1_{[i]0} + \Delta x \sum_\beta (\tilde{b}_\beta - \tilde{a}'_{\alpha\beta}) Y^{i\beta} = \pi^1_{[i]0} + \Delta x \sum_\beta \underbrace{\frac{\tilde{b}_\beta \tilde{b}_\alpha - \tilde{b}_\beta \tilde{a}_{\beta\alpha}}{\tilde{b}_\alpha}}_{\equiv \tilde{a}^{(2)}_{\alpha\beta}} Y^{i\beta}.$$

To summarize, our method is

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha}, \tag{2.15a}$$

$$P^0_{i\alpha} = \pi^0_{0[\alpha]} + \Delta t \sum_j a^{(2)}_{ij} X^{j\alpha}, \tag{2.15b}$$

$$\varphi_{1[\alpha]} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}, \tag{2.15c}$$

$$\pi^0_{1[\alpha]} = \pi^0_{0[\alpha]} + \Delta t \sum_j b_j X^{j\alpha}, \tag{2.15d}$$

$$\Phi_{i\alpha} = \tilde{\Phi}_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta} \tag{2.15e}$$

$$P^1_{i\alpha} = \pi^1_{[i]0} + \Delta x \sum_\beta \tilde{a}^{(2)}_{\alpha\beta} Y^{i\beta}, \tag{2.15f}$$

$$\varphi_{[i]1} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}, \tag{2.15g}$$

$$\pi^1_{[i]1} = \pi^1_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta Y^{i\beta}. \tag{2.15h}$$

$$V^{i\alpha} = \frac{\partial H}{\partial p^0}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.15i}$$

$$W^{i\alpha} = \frac{\partial H}{\partial p^1}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.15j}$$

$$X^{i\alpha} + Y^{i\alpha} = -\frac{\partial H}{\partial \phi}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.15k}$$

where $a^{(2)}_{ij} = \frac{b_j b_i - b_j a_{ji}}{b_i}$ and $\tilde{a}^{(2)}_{\alpha\beta} = \frac{\tilde{b}_\beta \tilde{b}_\alpha - \tilde{b}_\beta \tilde{a}_{\beta\alpha}}{\tilde{b}_\alpha}$. This is the usual form of a multisymplectic partitioned Runge–Kutta method. Note that our choice of $a^{(2)}_{ij}$ and $\tilde{a}^{(2)}_{\alpha\beta}$ (or equivalently our choice of $a'_{ij}, \tilde{a}'_{\alpha\beta}$) is the usual choice for the coefficients in the momenta expansion for a partitioned Runge–Kutta method to be multisymplectic (see, for example, Hong et al. [18], Reich [33], Ryland et al. [35]). Interestingly, however, from our perspective, our method based on the discrete boundary Hamiltonian is guaranteed to be multisymplectic so we had to impose no such conditions on the coefficients to ensure multisymplecticity; rather, the conditions for the coefficients arose from the necessity of the method to be well-defined, i.e., that the expansions of the field and momenta boundary values agreed with the discrete forward Hamilton's equations.

Remark 2.6. *In the above construction, we saw that the Runge–Kutta matrices (a_{ij}) and $(\tilde{a}_{\alpha\beta})$ were required to be invertible. We can see this directly from the internal stage expansions*

$$\Phi_{i\alpha} = \varphi_{0[\alpha]} + \Delta t \sum_j a_{ij} V^{j\alpha},$$
$$\tilde{\Phi}_{i\alpha} = \varphi_{[i]0} + \Delta x \sum_\beta \tilde{a}_{\alpha\beta} W^{i\beta},$$

since only when (a_{ij}) and $(\tilde{a}_{\alpha\beta})$ are invertible is extremizing K over $V^{i\alpha}$ and $W^{i\alpha}$ equivalent to extremizing K over $\Phi_{i\alpha}$ and $\tilde{\Phi}_{i\alpha}$, respectively. In the case of non-invertible Runge–Kutta matrices, the internal stages $\Phi_{i\alpha}$ and $\tilde{\Phi}_{i\alpha}$ do not depend independently on all of the $V^{i\alpha}$, $W^{i\alpha}$. For collocation Runge–Kutta methods, non-invertibility arises from the choice of the first quadrature point $c_1 = 0$. In our construction, if we choose $c_1 = 0$, then we are specifying an internal stage at a quadrature point where the field boundary value φ_A is already specified; thus, the internal stage at this point is not free to extremize over. Hence, in the non-invertible case, one has to use the specified boundary values to eliminate the degeneracy in the internal variables $V^{i\alpha}$ and $W^{i\alpha}$, reducing the number of internal variables to an independent subcollection of internal variables. Subsequently, one extremizes only over this independent subcollection of internal variables.

Momenta Internal Stages. In the above construction, we saw that we had to enforce consistency conditions on the momenta expansion coefficients in order for the method (2.15a)-(2.15k) to be well-defined. The issue is that we over-constrained the form of the momenta internal stages via our particular choice of expansion, since ultimately our goal was to derive the class of multisymplectic partitioned Runge–Kutta methods within our variational framework. One can avoid this problem altogether by working directly with the momenta internal stages $P^0_{i\alpha}$ and $P^1_{i\alpha}$ instead of the internal variables $X^{i\alpha}$ and $Y^{i\alpha}$, although the method will not ultimately be in the form of a multisymplectic partitioned Runge–Kutta method. This is possible for the momenta internal stages since the action does not depend on the derivatives of the momenta, unlike the field variable. We outline this procedure.

Assume the same expansions of $\Phi_{i\alpha}, \tilde{\Phi}_{i\alpha}, \varphi_{1[\alpha]}, \varphi_{[i]1}$ in terms of $\{V^{i\alpha}\}$ and $\{W^{i\alpha}\}$. For the momenta, we work directly with the internal stages $P^0_{i\alpha}$, $P^1_{i\alpha}$ instead of using an expansion. In this case, K is

$$\begin{aligned} K(\{\varphi_A, \pi_B, V^{i\alpha}, W^{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}, \lambda_{i\alpha}\}) = \Delta x \sum_\alpha \tilde{b}_\alpha \pi^0_{1[\alpha]}(\varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha}) \\ + \Delta t \sum_i b_i \pi^1_{[i]1}(\varphi_{[i]0} + \Delta x \sum_\beta \tilde{b}_\beta W^{i\beta}) \\ - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha P^0_{i\alpha} V^{i\alpha} - \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha P^1_{i\alpha} W^{i\alpha} \end{aligned}$$

$$+ \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha H(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \sum_{i,\alpha} \lambda_{i\alpha}(\Phi_{i\alpha} - \tilde{\Phi}_{i\alpha}).$$

H^+_d is obtained by extremizing K over the internal variables, $\{V^{i\alpha}, W^{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}, \lambda_{i\alpha}\}$.

The stationarity condition $\partial K/\partial P^0_{i\alpha} = 0$ (divided by $\Delta t \Delta x b_i \tilde{b}_\alpha$) gives

$$V^{i\alpha} = \frac{\partial H}{\partial p^0}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

Similarly, the stationarity condition $\partial K/\partial P^1_{i\alpha} = 0$ (divided by $\Delta t \Delta x b_i \tilde{b}_\alpha$) gives

$$W^{i\alpha} = \frac{\partial H}{\partial p^1}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}).$$

The stationarity condition $\partial K/\partial \lambda_{i\alpha} = 0$ gives $\Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$. The stationarity conditions $\partial K/\partial V^{j\beta} = 0$ and $\partial K/\partial W^{j\beta} = 0$ give respectively

$$\Delta t \Delta x b_j \tilde{b}_\beta (\pi^0_{1[\beta]} - P^0_{j\beta}) + \Delta t^2 \Delta x \sum_i b_i \tilde{b}_\beta a_{ij} \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}) + \Delta t \sum_i \lambda_{i\beta} a_{ij} = 0,$$

$$\Delta t \Delta x b_j \tilde{b}_\beta (\pi^1_{[j]1} - P^1_{j\beta}) + \Delta x^2 \Delta t \sum_\alpha b_j \tilde{b}_\alpha \tilde{a}_{\alpha\beta} (1-\theta) \frac{\partial H}{\partial \phi}(\tilde{\Phi}_{j\alpha}, P^0_{j\alpha}, P^1_{j\alpha}) - \Delta x \sum_\alpha \lambda_{j\alpha} \tilde{a}_{\alpha\beta} = 0.$$

Performing the same procedure we used to combine equations (2.11) and (2.12) to eliminate θ and the Lagrange multipliers, these two stationarity conditions can be combined to give

$$\sum_\beta b_j \tilde{b}_\beta \tilde{a}_{\beta\delta} \frac{(\pi^0_{1[\beta]} - P^0_{j\beta})}{\Delta x} + \sum_i b_i \tilde{b}_\delta a_{ij} \frac{(\pi^1_{[i]1} - P^1_{i\delta})}{\Delta t} = -\sum_{i,\beta} b_i \tilde{b}_\beta a_{ij} \tilde{a}_{\beta\delta} \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\beta}, P^0_{i\beta}, P^1_{i\beta}).$$

This combined condition, together with the other stationarity conditions $V^{i\alpha} = \partial H/\partial p^0(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})$, $W^{i\alpha} = \partial H/\partial p^1(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})$, and $\Phi_{i\alpha} = \tilde{\Phi}_{i\alpha}$ (ranging over all free indices) can be used to solve for the collection of internal variables $\{V^{i\alpha}, W^{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}\}_{i,\alpha}$ in terms of the supplied boundary data.

To conclude, we compute the discrete forward Hamilton's equations. For the field boundary values,

$$\varphi_{1[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \pi^0_{1[\alpha]}} = \varphi_{0[\alpha]} + \Delta t \sum_j b_j V^{j\alpha},$$

$$\varphi_{[i]1} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \pi^1_{[i]1}} = \varphi_{[i]0} + \Delta x \sum_\beta b_\beta W^{i\beta}.$$

Note that these equations already agree with the field expansion. For the momenta boundary values,

$$\pi^0_{0[\alpha]} = \frac{1}{\tilde{b}_\alpha \Delta x} \frac{\partial K}{\partial \varphi_{0[\alpha]}} = \pi^0_{1[\alpha]} + \Delta t \sum_i b_i \theta \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) + \frac{1}{\tilde{b}_\alpha \Delta x} \sum_i \lambda_{i\alpha},$$

$$\pi^1_{[i]0} = \frac{1}{b_i \Delta t} \frac{\partial K}{\partial \varphi_{[i]0}} = \pi^1_{[i]1} + \Delta x \sum_\alpha \tilde{b}_\alpha (1-\theta) \frac{\partial H}{\partial \phi}(\Phi^\theta_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) - \frac{1}{b_i \Delta t} \sum_\alpha \lambda_{i\alpha}.$$

As we did before for the partitioned Runge–Kutta method, we can act on the stationarity conditions $\partial K/\partial V^{j\beta} = 0 = \partial K/\partial W^{j\beta}$ by the inverses of the Runge–Kutta matrices to solve for the Lagrange multipliers and substitute them into the discrete forward Hamilton's equations for the momenta, ultimately eliminating θ and the Lagrange multipliers. The discrete forward Hamilton's equations for the momenta are then

$$\pi^0_{0[\alpha]} = \pi^0_{1[\alpha]} - \Delta t \sum_{j,l} b_j (a^{-1})_{jl} \frac{\pi^0_{1[\alpha]} - P^0_{j\alpha}}{\Delta x},$$

$$\pi^1_{[i]0} = \pi^1_{[i]1} - \Delta x \sum_{\alpha,\beta} \tilde{b}_\alpha (\tilde{a}^{-1})_{\alpha\beta} \frac{\pi^1_{[i]1} - P^1_{i\alpha}}{\Delta t}.$$

Hence, by working with the internal stages for the momenta directly, as opposed to utilizing an expansion, we see that the method we derived is already well-defined (and also automatically multisymplectic), although it is not directly in the form of a multisymplectic partitioned Runge–Kutta method.

These various approaches demonstrate the versatility of our variational framework; once one chooses an approximation for the fields, its derivatives, and the momenta (as well as some approximation for the various integrals involved), one can construct the discrete boundary Hamiltonian and subsequently the variational framework produces a multisymplectic integrator. If one over-constrains the form of the momenta expansion, as opposed to using the internal stages directly, one must also check whether the method is well-defined. Another approach that is possible within this framework is to discretize at the level of the field using some (possibly non-tensor product) function space and subsequently take derivatives of the basis functions to obtain an approximation of the derivatives of the fields. For example, we expect that utilizing spectral element bases to discretize at the level of the field within our framework will produce multisymplectic spectral discretizations like those obtained in Bridges and Reich [7], Islas and Schober [19, 20]. Another interesting application of our construction would be to construct multisymplectic discretizations of the total exterior algebra bundle (see Bridges and Reich [8]) using Galerkin discretizations arising from the Finite Element Exterior Calculus framework (Arnold et al. [2, 3], Hiptmair [16]), allowing one to discretize Hamiltonian PDEs with more general configuration bundles.

2.4. **Multisymplecticity Revisited.** Now, we discuss in what sense the discrete multisymplectic form formula (2.4) corresponds to our discretization of the field equations. Consider the integral form of the De Donder–Weyl equations over $\Box = [0, \Delta t] \times [0, \Delta x]$,

$$\int_\Box \Big(\partial_\mu p^\mu + \frac{\partial H}{\partial \phi}(\phi, p^0, p^1) \Big) d^2x = 0, \tag{2.16a}$$

$$\int_\Box \Big(\partial_0 \phi - \frac{\partial H}{\partial p^0}(\phi, p^0, p^1) \Big) d^2x = 0., \tag{2.16b}$$

$$\int_\Box \Big(\partial_1 \phi - \frac{\partial H}{\partial p^1}(\phi, p^0, p^1) \Big) d^2x = 0. \tag{2.16c}$$

Applying our quadrature approximation to equation (2.16a),

$$\begin{aligned} 0 &= \int_0^{\Delta t} \int_0^{\Delta x} \Big(\partial_0 p^0 + \partial_1 p^1 + \frac{\partial H}{\partial \phi}(\phi, p^0, p^1) \Big) dx dt \\ &= \int_0^{\Delta x} (p^0|_{t=\Delta t} - p^0|_{t=0}) dx + \int_0^{\Delta t} (p^1|_{x=\Delta x} - p^0|_{x=0}) dt + \int_0^{\Delta t} \int_0^{\Delta x} \frac{\partial H}{\partial \phi}(\phi, p^0, p^1) dx dt \\ &\approx \Delta x \sum_\alpha \tilde{b}_\alpha (p^0|_{(\Delta t, \tilde{c}_\alpha \Delta x)} - p^0|_{(0, \tilde{c}_\alpha \Delta x)}) + \Delta t \sum_i b_i (p^1|_{(c_i \Delta t, \Delta x)} - p^1|_{(c_i \Delta t, 0)}) \end{aligned}$$

$$+ \Delta t \Delta x \sum_{i,\alpha} \frac{\partial H}{\partial \phi}(\phi, p^0, p^1)|_{(c_i\Delta t, \tilde{c}_\alpha \Delta x)}.$$

Consider the multisymplectic partitioned Runge–Kutta method (2.15a)-(2.15k); if we multiply equation (2.15d) by $\tilde{b}_\alpha$ and sum over α, multiply equation (2.15h) by b_i and sum over i, and add the resulting equations together, we have

$$0 = \Delta x \sum_\alpha \tilde{b}_\alpha(\pi^0_{1[\alpha]} - \pi^1_{0[\alpha]}) + \Delta t \sum_i b_i(\pi^1_{[i]1} - \pi^1_{[i]0}) + \Delta t \Delta x \sum_{i,\alpha} b_i \tilde{b}_\alpha \frac{\partial H}{\partial \phi}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}), \tag{2.17}$$

where we used $X^{i\alpha} + Y^{i\alpha} = \partial H/\partial\phi(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha})$. Comparing these two, we see that the discrete method satisfies an approximation of the integral form of the De Donder–Weyl equation (2.16a) and that the error in the approximation of the field equations is directly related to the quadrature error and the field and momenta expansions. Similar statements can be made about the other De Donder–Weyl equations, (2.16b) and (2.16c).

Now, let's write our approximation (2.17) of the integral De Donder–Weyl equations as a difference equation. For a quantity f defined on the nodes of the edges $\{0\} \times [0, \Delta x]$ and $\{\Delta t\} \times [0, \Delta x]$ (and similarly a quantity g defined on the nodes of the edges $[0, \Delta t] \times \{0\}$ and $[0, \Delta t] \times \{\Delta x\}$), define

$$\delta^0_{[\alpha]} f = f_{1[\alpha]} - f_{0[\alpha]},$$
$$\delta^1_{[i]} g = g_{[i]1} - g_{[i]0}.$$

Define the discrete difference operators

$$\partial^\Box_0 = \frac{1}{\Delta t} \sum_\alpha \tilde{b}_\alpha \delta^0_{[\alpha]},$$
$$\partial^\Box_1 = \frac{1}{\Delta x} \sum_i b_i \delta^1_{[i]}.$$

Dividing equation (2.17) by $\Delta t \Delta x$, we see that it satisfies

$$\partial^\Box_0 \pi^0 + \partial^\Box_1 \pi^1 = -\sum_{i\alpha} b_i \tilde{b}_\alpha \frac{\partial H}{\partial \phi}(\Phi_{i\alpha}, P^0_{i\alpha}, P^1_{i\alpha}) \equiv -\Big\langle \frac{\partial H}{\partial \phi} \Big\rangle_\Box,$$

where $\langle \frac{\partial H}{\partial \phi} \rangle_\Box$ denotes our quadrature approximation of the average value of $\partial H/\partial\phi$ on $\Box$. Similarly, the other discrete equations satisfy

$$\partial^\Box_0 \varphi = \Big\langle \frac{\partial H}{\partial p^0} \Big\rangle_\Box,$$
$$\partial^\Box_1 \varphi = \Big\langle \frac{\partial H}{\partial p^1} \Big\rangle_\Box.$$

These difference equations correspond to our discretization of (the integral form) of the DDW equations $\partial_0 p^0 + \partial_1 p^1 = -\partial H/\partial\phi$, $\partial_\mu \phi = \partial H/p^\mu$. As mentioned in Section 1.3, a method is called multisymplectic if the difference operators used in the discretization of the field equations are the same difference operators which appear in the discrete multisymplectic form formula that the method admits. In our case, if we divide the discrete multisymplectic form formula (2.4) by $\Delta t \Delta x$, we see that it satisfies

$$\partial^\Box_0 \omega^0 + \partial^\Box_1 \omega^1 = 0$$

(when evaluated on discrete first variations), where $\omega^0 = d\varphi \wedge d\pi^0, \omega^1 = d\varphi \wedge d\pi^1$. Hence, our method is multisymplectic in the sense that the difference operators which appear in the difference equation that the discrete solution satisfies over $\Box \in \mathcal{T}(X)$ are the same difference operators which appear in the discrete multisymplectic form formula.

3. Conclusion and Future Directions

In this paper, we extended the construction of Hamiltonian variational integrators to the setting of multisymplectic Hamiltonian PDEs. Our construction is based on a discrete approximation of the boundary Hamiltonian, introduced in Vankerschaver et al. [39]. Through the Type II variational principle, this discrete boundary Hamiltonian is a generating function for the discrete Hamilton's equations that define our multisymplectic integrator. The discrete variational principle automatically yields integrators which are multisymplectic and satisfy a discrete Noether's theorem for group-invariant discretizations. As an application of this variational framework, we derived the class of multisymplectic partitioned Runge–Kutta methods; however, our construction is more general and is not limited to this class of multisymplectic integrators. Finally, we showed that the discrete multisymplecticity which arose from the discrete variational principle agrees with the notion of discrete multisymplecticity introduced in Bridges and Reich [6].

Perhaps the most natural research direction is to establish a variational error analysis result which demonstrates that a computable discrete Hamiltonian that approximates the boundary Hamiltonian to a given order of accuracy will result in a numerical method for the Hamiltonian partial differential equation with the same order of accuracy. It should be observed that this poses two main challenges as compared to the case for ordinary differential equations. The first is that the boundary of the spacetime domain is in general curved, and the space of boundary data (and boundary momentum) is infinite-dimensional. As such, one would first have to approximate the spacetime domain with a spacetime mesh, and choose a finite-dimensional subspace for sections of the dual jet bundle that is subordinate to this spacetime mesh. Then, the error between the computable discrete Hamiltonian and the boundary Hamiltonian can be decomposed into three terms, the first of which can be bounded by assuming that the boundary-value problem is well-posed and therefore has continuous dependence on the boundary data, the second is associated with the variational crime of replacing the spacetime domain with a spacetime mesh, and the third is a term that is analogous to what arises in the usual variational error analysis for ordinary differential equations.

The second natural direction would be to establish a quasi-optimality result which demonstrates that the variational error in the construction of a Galerkin boundary Hamiltonian is bounded from above by a multiple of the best approximation error of the finite-dimensional function space used to approximate sections of the configuration bundle.

Finally, it was established in McLachlan and Stern [30] that many hybridizable discontinuous Galerkin methods are multisymplectic when applied to semilinear elliptic PDEs in mixed form, and it would be interesting to see the kind of multisymplectic Hamiltonian variational integrators that would arise for Hamiltonian time-evolution PDEs when using spacetime discontinuous Galerkin finite element spaces to discretize the dual jet bundle.

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