

Multisymplectic Lie group variational integrators

Part 1: derivation and properties

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Abstract—Multisymplectic variational integrators are structure preserving numerical schemes especially designed for PDEs derived from covariant spacetime Hamilton principles. The present note summarizes some results obtained in our paper [2]. We present a class of multisymplectic variational integrators for mechanical systems on Lie groups. The multisymplectic scheme is derived by applying a discrete version of the spacetime covariant Hamilton principle. The Lie group structure is used to rewrite the discrete variational principle in a trivialized formulation which allows us to make use of the vector space structure of the Lie algebra. Some aspects of the symplectic character of the discrete temporal and spatial evolution are given.

Index Terms—multisymplectic structure, discrete mechanics, variational integrator, Lie group symmetry, discrete momentum map, discrete global Noether theorem

I. INTRODUCTION AND PRELIMINARIES

Multisymplectic variational integrators are structure preserving numerical schemes designed for solving PDEs arising from covariant Euler-Lagrange equations. These schemes are derived from a discrete version of the covariant Hamilton principle of field theory and preserve, at the discrete level, the associated multisymplectic geometry.

Multisymplectic variational integrators can be seen as the spacetime generalization of the well-known variational integrators for classical mechanics (see [10]). Recall that the discrete Lagrangian flow obtained through a classical variational integrator preserves a symplectic form. From this property, it follows, by backward error analysis, that the energy is approximately preserved. For multisymplectic integrators, however, the situation is much more involved, the analogue of the symplectic property being given by a *discrete version of the multisymplectic form formula* (see [9]). This formula is the spacetime analogue of the symplectic property of the discrete flow associated to variational integrators in time. The continuous multisymplectic form formula is a property of the solution of the covariant Euler-Lagrange equations in field theory, see [6] to which we refer for the multisymplectic geometry of classical field theory.

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A. Classical and covariant Euler-Lagrange equations

In classical mechanics, the Euler-Lagrange equations associated to a Lagrangian $L : TQ \rightarrow \mathbb{R}$ are obtained by computing the critical curves $q : [0, T] \rightarrow Q$ of the action functional $\mathfrak{S}(q) = \int_0^T L dt$ among curves with prescribed endpoint values:

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \int_0^T L(q_\varepsilon(t), \dot{q}_\varepsilon(t)) dt = 0, \quad q_\varepsilon(0) = q_0, \quad q_\varepsilon(T) = q_T.$$

In field theory, curves are replaced by sections of a fiber bundle $\pi : Y \rightarrow X$. We shall consider the special case of the trivial fiber bundle $\pi : Y = X \times Q \rightarrow X$, where $X = [0, T] \times [0, L] \ni (t, s)$, so that the sections are identified with maps $q : [0, T] \times [0, L] \rightarrow Q$. The Lagrangian is defined on the first jet bundle $J^1Y \rightarrow Y$ of $\pi : Y \rightarrow X$, identified in our special case with the vector bundle $L(TX, TQ) \rightarrow X \times Q$ whose fiber at (x, q) is the vector space of all linear maps $T_x X \rightarrow T_q Q$. Given a Lagrangian $\mathcal{L} : L(TX, TQ) \rightarrow \mathbb{R}$, the covariant Euler-Lagrange equations are obtained similarly as before by computing the critical maps of the action functional $\mathfrak{S}(q) = \int_0^T \int_0^L \mathcal{L} dt ds$ among maps with prescribed values on ∂X :

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \int_0^T \int_0^L \mathcal{L}(q_\varepsilon(t, s), \partial_t q_\varepsilon(t, s), \partial_s q_\varepsilon(t, s)) dt ds = 0, \quad (1)$$

$$q_\varepsilon|_{\partial X}(t, s) = q_\partial(t, s),$$

where $q_\partial : \partial X \rightarrow Q$ is given.

It is well-known that if L is regular, the flow of the Euler-Lagrange equations is symplectic relative to the symplectic form Ω_L on TQ obtained by pulling back the canonical symplectic form on T^*Q by the Legendre transform of L . The field theoretic generalization of this fact is given by the *multisymplectic form formula*, see [9].

B. Discrete Euler-Lagrange equations and (multi-) symplecticity

The variational discretization of the classical Euler-Lagrange equation is obtained by replacing the curve with a sequence of points (discrete curve) $q_d : \{t^j = j\Delta t\}_{j=0}^N \rightarrow Q$, $q^j := q_d(t^j)$, where Δt is the time step, and by considering a discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ which we think of as approximating the action integral of L along the curve segment between q^j and q^{j+1} . The *discrete Euler-Lagrange (DEL) equations* are obtained by computing the critical points of the discrete action functional $\mathfrak{S}_d(q_d) := \sum_{j=0}^{N-1} L_d(q^j, q^{j+1})$ among discrete curves with prescribed endpoint values. The

resulting discrete flow $(q^{j-1}, q^j) \mapsto (q^j, q^{j+1})$, is *symplectic* relative to the symplectic form Ω_{L_d} on $Q \times Q$ obtained by pulling back the canonical symplectic form on T^*Q by the discrete Legendre transform of L_d , see [10].

Similarly, the variational discretization of the covariant Euler-Lagrange equation is obtained by applying a discrete version of the variational principle (1) for an appropriate discretization of X and \mathcal{L} . In our case, we choose the discretization of $X = [0, T] \times [0, L]$ given by the set of nodes $X_d = \{(j, a) \in \mathbb{Z} \times \mathbb{Z} \mid j = 0, \dots, N-1, a = 0, \dots, A-1\}$ and the set X_d^Δ of elemental subsets given by triangles $\Delta_a^j = ((j, a), (j+1, a), (j, a+1))$. A discrete map reads $q_d : X^d \rightarrow Q$, $q_a^j := q_d(j, a)$. Once a discrete Lagrangian

$$\mathcal{L}_d = \mathcal{L}_d(\Delta_a^j, q_a^j, q_a^{j+1}, q_{a+1}^j) : X_d^\Delta \times Q \times Q \times Q \rightarrow \mathbb{R}$$

has been chosen, the *discrete covariant Euler-Lagrange (DCEL) equations* are obtained by computing the critical points of the discrete action functional

$$\mathfrak{S}_d(q_d) := \sum_{j=0}^{N-1} \sum_{a=0}^{A-1} \mathcal{L}_d(\Delta_a^j, q_a^j, q_a^{j+1}, q_{a+1}^j),$$

among discrete maps with prescribed boundary values. The resulting discrete scheme is *multisymplectic* in the sense that it verifies a discrete version of the multisymplectic form formula, see [9].

II. COVARIANT EULER-LAGRANGE EQUATIONS ON LIE GROUPS

We now consider the special case when the configuration space Q is a Lie group G . This allows us to trivialize the Lagrangian and the equations by using the diffeomorphism $v_g \in TG \rightarrow (g, g^{-1}v_g) \in G \times \mathfrak{g}$, where \mathfrak{g} denotes the Lie algebra of G . For example, given a Lagrangian $\mathcal{L} : L(TX, TG) \rightarrow \mathbb{R}$, since $X = [0, T] \times [0, L]$, its trivialization is $\bar{\mathcal{L}} : G \times \mathfrak{g} \times \mathfrak{g} \rightarrow \mathbb{R}$ defined by $\mathcal{L}(g, \dot{g}, g') = \bar{\mathcal{L}}(g, \xi := g^{-1}\dot{g}, \eta := g^{-1}g')$. Using (1) and computing the variations of $\xi(t, s)$ and $\eta(t, s)$ induced from the variations of $g(t, s)$, we get the trivialized *covariant Euler-Lagrange equations* (CEL)

$$\frac{\partial}{\partial t} \frac{\delta \bar{\mathcal{L}}}{\delta \xi} + \frac{\partial}{\partial s} \frac{\delta \bar{\mathcal{L}}}{\delta \eta} = \text{ad}_\xi^* \frac{\delta \bar{\mathcal{L}}}{\delta \xi} + \text{ad}_\eta^* \frac{\delta \bar{\mathcal{L}}}{\delta \eta} + g^{-1} \frac{\partial \bar{\mathcal{L}}}{\partial g}. \quad (2)$$

A. Boundary conditions

If the field $g(t, s)$ has prescribed values only on the temporal boundary $\{0, T\} \times [0, L]$, then, in addition to (2), the covariant Hamilton principle also yields the *zero traction boundary conditions*

$$\frac{\delta \bar{\mathcal{L}}}{\delta \eta}(t, 0) = \frac{\delta \bar{\mathcal{L}}}{\delta \eta}(t, L) = 0, \quad \forall t. \quad (3)$$

Similarly, if the field $g(t, s)$ has prescribed values only on the spatial boundary $[0, T] \times \{0, L\}$, then the covariant Hamilton principle yields the *zero momentum boundary conditions*

$$\frac{\delta \bar{\mathcal{L}}}{\delta \xi}(0, s) = \frac{\delta \bar{\mathcal{L}}}{\delta \xi}(T, s) = 0, \quad \forall s. \quad (4)$$

B. Space and time evolutionary descriptions

According to the preferred point of view needed for the application, one can interpret the field $q(t, s) \in Q$ either as a time-evolutionary curve $t \mapsto q(t) \in \mathcal{F}([0, L], Q)$ or as a spatial-evolutionary curve $s \mapsto q(s) \in \mathcal{F}([0, T], Q)$, by writing $q(t, s) = q(s)(t)$ or $q(t, s) = q(t)(s)$. From this, one can define the two classical Lagrangians

$$\mathbb{L}(q(t), \dot{q}(t)) := \int_0^L \mathcal{L}(q(t, s), \dot{q}(t, s), \partial_s q(t, s)) ds$$

and

$$\mathbb{N}(q(s), q'(s)) := \int_0^T \mathcal{L}(q(t, s), \partial_t q(t, s), q'(t, s)) dt.$$

Let us now comment on the link between the CEL equations for \mathcal{L} and the classical EL equations for \mathbb{L} and \mathbb{N} .

– If the field has prescribed values only on the temporal boundary, then one can consider the EL equations for \mathbb{L} on $T\mathcal{F}([0, L], Q)$ and they turn out to be equivalent to the CEL for \mathcal{L} together with zero traction boundary conditions ((3) if $Q = G$). However, the Lagrangian \mathbb{N} has to be considered on $T\mathcal{F}^0([0, T], Q)$, where $\mathcal{F}^0([0, T], Q)$ denotes the space of fields that verify the prescribed boundary conditions at $t = 0, T$, in which case these boundary conditions must be independent on the variable s . The EL equations for \mathbb{N} yield the CEL equations, whereas the zero momentum boundary conditions ((4) if $Q = G$) come from the fact that endpoints conditions are not prescribed when applying Hamilton principle to \mathbb{N} .

– If the field has prescribed values only on the spatial boundary, then we have the reverse situation as the one described above. In particular, \mathbb{L} is now defined on the tangent bundle to $\mathcal{F}_0([0, L], Q)$ which consists of fields that verify the prescribed boundary conditions at $s = 0, L$, in which case these boundary conditions must be independent on the time t .

C. The case of Lie groups

When $Q = G$ then, in a similar way with \mathcal{L} earlier, one can associate to \mathbb{L} and \mathbb{N} the trivialized expressions $\bar{\mathbb{L}} = \bar{\mathbb{L}}(g, \xi) : \mathcal{F}([0, L], G \times \mathfrak{g}) \rightarrow \mathbb{R}$ and $\bar{\mathbb{N}} = \bar{\mathbb{N}}(g, \eta) : \mathcal{F}([0, T], G \times \mathfrak{g}) \rightarrow \mathbb{R}$ and the trivialized EL equations read

$$\frac{d}{dt} \frac{\partial \bar{\mathbb{L}}}{\partial \xi} = \text{ad}_\xi^* \frac{\partial \bar{\mathbb{L}}}{\partial \xi} + g^{-1} \frac{\partial \bar{\mathbb{L}}}{\partial g}$$

resp.,

$$\frac{d}{dt} \frac{\partial \bar{\mathbb{N}}}{\partial \eta} = \text{ad}_\eta^* \frac{\partial \bar{\mathbb{N}}}{\partial \eta} + g^{-1} \frac{\partial \bar{\mathbb{N}}}{\partial g}.$$

D. The G -invariant case: covariant Euler-Poincaré equations and G -strands

When the Lagrangian \mathcal{L} is G -invariant, the CEL equations (2) yield the *covariant Euler-Poincaré equations* (CEP)

$$\frac{\partial}{\partial t} \frac{\delta \bar{\mathcal{L}}}{\delta \xi} + \frac{\partial}{\partial s} \frac{\delta \bar{\mathcal{L}}}{\delta \eta} = \text{ad}_\xi^* \frac{\delta \bar{\mathcal{L}}}{\delta \xi} + \text{ad}_\eta^* \frac{\delta \bar{\mathcal{L}}}{\delta \eta}, \quad (5)$$

also called G -strand equations ([8]) since they are useful for description of strands and beams when $G = SE(3)$, see [3]. One passes from the CEL equations to the CEP

equations via the process of covariant Euler-Poincaré reduction ([1]). As explained in [4], one can also obtain the CEP by using a classical (as opposed to covariant) Lagrangian reduction process. In this case, one interprets $g(t, s)$ as a time evolutionary curve $t \mapsto g(t) \in \mathcal{F}([0, L], G)$ and the needed reduction process is the *affine Euler-Poincaré reduction* with cocycle ([5]) applied to the infinite dimensional Lie group $\mathcal{F}([0, L], G)$. The same point of view can be applied for the spatial evolution, by interpreting $g(t, s)$ as a space evolutionary curve $s \mapsto g(s) \in \mathcal{F}([0, T], G)$.

III. MULTISYMPLECTIC INTEGRATORS FOR CEL ON LIE GROUPS

As we explained earlier, the discrete CEL are obtained by computing the critical points of the discrete action functional $\mathfrak{S}_d(q_d) := \sum_{j=0}^{N-1} \sum_{a=0}^{A-1} \mathcal{L}_d(\Delta_a^j, q_a^j, q_{a+1}^{j+1}, q_{a+1}^j)$. In the special case $Q = G$, one takes advantage of the Lie group structure to consider the discrete trivialized Lagrangian $\bar{\mathcal{L}}_d : X^\Delta \times G \times \mathfrak{g} \times \mathfrak{g} \rightarrow \mathbb{R}$ defined by

$$\bar{\mathcal{L}}_d(\Delta_a^j, g_a^j, \xi_a^j, \eta_a^j) := \mathcal{L}_d(\Delta_a^j, g_a^j, g_a^{j+1}, g_{a+1}^j),$$

where $\xi_a^j := \tau^{-1}((g_a^j)^{-1} g_a^{j+1})/\Delta t$ and $\eta_a^j := \tau^{-1}((g_a^j)^{-1} g_{a+1}^j)/\Delta s$ are defined with the help of a given local diffeomorphism $\tau : \mathfrak{g} \rightarrow G$ in a neighborhood of the identity, such that $\tau(0) = e$.

A. Discrete CEL on Lie groups

By computing the constrained variations of ξ_a^j and η_a^j induced by free variations of g_a^j , one obtains from $\delta \mathfrak{S}_d(q_d) = 0$ the *discrete CEL equations on Lie groups*

$$\begin{aligned} & \frac{1}{\Delta t} (\mu_a^j - \text{Ad}_{\tau(\Delta t \xi_a^{j-1})}^* \mu_a^{j-1}) \\ & + \frac{1}{\Delta s} (\lambda_a^j - \text{Ad}_{\tau(\Delta s \eta_{a-1}^j)}^* \lambda_{a-1}^j) = (g_a^j)^{-1} \frac{\partial \bar{\mathcal{L}}_d}{\partial g_a^j}, \end{aligned} \quad (6)$$

for all $j = 1, \dots, N-1$ and $a = 1, \dots, A-1$, where the discrete momenta are defined by

$$\mu_a^j := (d^R \tau_{\Delta t \xi_a^j}^{-1})^* \frac{\partial \bar{\mathcal{L}}_d}{\partial \xi_a^j}, \quad \lambda_a^j := (d^R \tau_{\Delta s \eta_a^j}^{-1})^* \frac{\partial \bar{\mathcal{L}}_d}{\partial \eta_a^j},$$

where $d^R \tau_{\xi}^{-1} : \mathfrak{g} \rightarrow \mathfrak{g}$ denotes the right trivialized derivative of $\tau^{-1} : G \rightarrow \mathfrak{g}$ at $g := \tau(\xi)$.

B. Discrete boundary conditions

The discrete variational approach also yields a consistent discretization of the boundary conditions (3) and (4). The discrete zero momentum boundary condition reads

$$\begin{aligned} & \frac{1}{\Delta t} (\mu_0^j - \text{Ad}_{\tau(\Delta t \xi_0^{j-1})}^* \mu_0^{j-1}) + \frac{1}{\Delta s} \lambda_0^j = (g_0^j)^{-1} \frac{\partial \bar{\mathcal{L}}_d}{\partial \xi_0^j}, \\ & \text{Ad}_{\tau(\Delta s \eta_{A-1}^j)}^* \lambda_{A-1}^j = 0, \end{aligned}$$

for all $j = 1, \dots, N-1$, and the discrete zero momentum boundary condition reads

$$\begin{aligned} & \frac{1}{\Delta t} \mu_a^0 + \frac{1}{\Delta s} (\lambda_a^0 - \text{Ad}_{\tau(\Delta s \eta_{a-1}^0)}^* \lambda_{a-1}^0) = (g_a^0)^{-1} \frac{\partial \bar{\mathcal{L}}_d}{\partial \xi_a^0}, \\ & \text{Ad}_{\tau(\Delta t \xi_a^{N-1})}^* \mu_a^{N-1} = 0, \end{aligned}$$

for all $a = 1, \dots, A-1$.

C. Discrete temporal and spatial evolution

In complete analogy with the definition of the evolutionary Lagrangian $\bar{\mathcal{L}}$ and $\bar{\mathcal{N}}$, we can define the discrete Lagrangians

$$\begin{aligned} \bar{\mathcal{L}}_d(\mathbf{g}^j, \boldsymbol{\xi}^j) &= \sum_{a=0}^{A-1} \bar{\mathcal{L}}_d(\Delta_a^j, g_a^j, \xi_a^j, \eta_a^j), \\ \bar{\mathcal{N}}_d(\mathbf{g}_a, \boldsymbol{\eta}_a) &= \sum_{j=0}^{N-1} \bar{\mathcal{L}}_d(\Delta_a^j, g_a^j, \xi_a^j, \eta_a^j), \end{aligned}$$

where we assumed that $\bar{\mathcal{L}}_d$ does not depend explicitly on the discrete time and discrete space coordinates. These discrete Lagrangians are associated to the discrete temporal evolution $\mathbf{g}^j = (g_0^j, \dots, g_A^j)$, $j = 0, \dots, N$ and spatial evolution $\mathbf{g}_a = (g_a^0, \dots, g_a^N)$, $a = 0, \dots, N$, where $\boldsymbol{\xi}^j := \frac{1}{\Delta t} \tau^{-1}((\mathbf{g}^j)^{-1} \mathbf{g}^{j+1}) \in \mathfrak{g}^{A+1}$ and $\boldsymbol{\eta}_a := \frac{1}{\Delta s} \tau^{-1}((\mathbf{g}_a)^{-1} \mathbf{g}_{a+1}) \in \mathfrak{g}^{N+1}$. The discrete CEL equations associated to $\bar{\mathcal{L}}_d$ and the discrete EL equations associated to $\bar{\mathcal{L}}_d$ and $\bar{\mathcal{N}}_d$ are related exactly as their continuous counterparts, as explained in §II-B. This relation depends on the imposed boundary conditions.

As mentioned earlier, the CEL (6) associated to $\bar{\mathcal{L}}_d$ yield a multisymplectic integrator. The interpretation of these equations as discrete EL equations associated to $\bar{\mathcal{L}}_d$, resp., $\bar{\mathcal{N}}_d$ allows us to study the symplecticity in time, resp., in space, of the numerical scheme. Of course, for such a study it is crucial to specify the prescribed boundary conditions.

D. G-invariant case

When the discrete covariant Lagrangian is G -invariant, i.e., $\bar{\mathcal{L}}_d(\Delta_a^j, g_a^j, \xi_a^j, \eta_a^j) = \ell_d(\Delta_a^j, \xi_a^j, \eta_a^j)$, then the discrete CEL (6) yield a discrete version of the CEP equations (or G -strand equations) (5). They are obtained simply by writing $\partial \bar{\mathcal{L}}_d / \partial g_a^j = 0$ in (6) and arise from a discrete covariant Lagrangian reduction by symmetry. Note that the discrete CEP equations for $\ell_d(\Delta_a^j, \xi_a^j, \eta_a^j)$ can also be interpreted as a symmetry reduced version of the discrete EL equations for $\mathcal{L}_d(\mathbf{g}^j, \mathbf{g}^{j+1})$. To a discrete spacetime covariant reduction for \mathcal{L}_d thus corresponds a discrete dynamic reduction for \mathcal{L}_d . The same comment applies to \mathcal{N}_d . It would be interesting to analyze the link between this observation and the approach carried out in [4] which relates, in the continuous case, the covariant and dynamic reductions in principal bundle field theories.

E. Covariant and classical momentum maps

One of the attractive property of multisymplectic integrators is that in presence of a symmetry of the Lagrangian, they allow for the definition of a discrete version of covariant momentum maps and they verify a discrete version of the covariant Noether theorem. As we have seen, the multisymplectic scheme (6) can also be written as a discrete (classical) EL equation for the discrete Lagrangians \mathcal{L}_d and \mathcal{N}_d . Therefore, the multisymplectic integrator also verifies a discrete version of the classical Noether theorem associated to the temporal or spatial evolution. The relation between the discrete covariant and classical Noether theorems depends however on the prescribed boundary conditions, as explained in details in [2].

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