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Variational integrators for non-autonomous Lagrangian systems

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ABSTRACT

Numerical methods that preserve geometric invariants of the system, such as energy, momentum or the symplectic form, are called geometric integrators. Variational integrators are an important class of geometric integrators. The general idea for those variational integrators is to discretize Hamilton's principle rather than the equations of motion in a way that preserves some of the invariants of the original system. In this paper we construct variational integrators with fixed time step for time-dependent Lagrangian systems modelling an important class of autonomous dissipative systems. These integrators are derived via a family of discrete Lagrangian functions each one for a fixed time-step. This allows to recover at each step on the set of discrete sequences the preservation properties of variational integrators for autonomous Lagrangian systems, such as symplecticity or backward error analysis for these systems. We also present a discrete Noether theorem for this class of systems.

1. Introduction

Since the emergence of computational methods, fundamental properties such as accuracy, stability, convergence, and computational efficiency have been considered crucial for deciding the utility of a numerical algorithm. Geometric numerical integrators are concerned with numerical algorithms that preserve the system's fundamental physics by keeping the geometric properties of the dynamical system under study. The key idea of the structure-preserving approach is to treat the numerical method as a discrete dynamical system which approximates the continuous-time flow of the governing continuous-time differential equation, instead of focusing on the numerical approximation of a single trajectory. Such an approach allows a better understanding of the invariants and qualitative properties of the numerical method. Using ideas from differential geometry, structure-preserving integrators have produced a variety of numerical methods for simulating systems described by ordinary differential equations preserving its qualitative features. In particular, numerical methods based on discrete variational principles [1,2] may exhibit superior numerical stability and structure-preserving capabilities than traditional integration schemes for ordinary differential equations.

Variational integrators are geometric numerical methods derived from the discretization of variational principles [1–3]. These integrators retain some of the main geometric properties of the continuous systems, such as preservation of the manifold structure at each step of the algorithm, symplecticity, momentum conservation (as long as the symmetry survives the discretization procedure), and a good behaviour of the energy function associated to the system for long

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time simulation steps. This class of numerical methods has been applied to a wide range of problems in optimal control [4–6], constrained systems [7], formation control of multi-agent systems [8], nonholonomic systems [9], accelerated optimization [10], flocking control [11] and motion planning for underactuated robots [12], among many others.

In this paper we construct variational integrators for non-autonomous Lagrangian systems with fixed time step (see [2] for variable time step). More precisely, a variational integrator for a time-dependent Lagrangian system is derived through a family of discrete Lagrangian functions each one for a fixed time-step (see [10,13]). This allows to recover at each step on the set of discrete sequences the preservation properties of variational integrators for autonomous Lagrangian systems such as symplecticity of the integrator or cosymplecticity of the modified time-dependent Hamiltonian system using backward error analysis. We also obtain a discrete-time Noether Theorem for the relation between symmetries and first integrals. Such a result allow us to guarantee, for instance, an exponentially fast rate of change for the linear and angular momentum of certain mechanical systems. The class of variational integrators developed in this work are motivated by the recent applications of geometric integrators in contact [14,15], celestial mechanics [16] and formation control of multi-agent systems [8,17,18].

The remainder of the paper is structured as follows. Section 2 introduces some geometric aspects of time-dependent Lagrangian systems, Noether symmetries, constants of the motion and its relation via a Noether Theorem for time-dependent Lagrangian systems. Section 3 constructs the variational integrator for time-dependent Lagrangian systems and the discrete-time version of Noether theorem. In Section 4 we derive the discrete Hamiltonian flow for discrete-time non-autonomous Hamiltonian Systems which is further employed in Section 5 in the context of the backward error analysis. An example is shown in Section 6. Conclusions are presented in Section 7.

2. Symmetries and constants of the motion for non-autonomous Lagrangian systems

Let Q be the configuration space of a mechanical system, that we will assume is a differentiable manifold of dimension n with local coordinates $q = (q^1, \dots, q^n)$. Let TQ be the tangent bundle of Q, locally described by positions and velocities, $(q^i, \dot{q}^i)$ with $\dim(TQ) = 2n$. Let T^*Q be its cotangent bundle, locally described by positions and momenta, (q^i, p_i) where also $\dim(T^*Q) = 2n$. The tangent and cotangent bundle at a point $q \in Q$ are denoted as T_qQ and T_q^*Q, respectively. We denote by $\tau_Q : TQ \to Q$ the canonical projection on the tangent bundle which in local coordinates is given by $\tau_Q(q^i, \dot{q}^i) = (q^i)$ and by $\pi_Q : T^*Q \to Q$ the canonical projection on the cotangent bundle, $\pi_Q(q^i, p_i) = (q^i)$.

Consider a time-dependent Lagrangian $L : \mathbb{R} \times TQ \to \mathbb{R}$, and denote by $\mathbb{F}L : \mathbb{R} \times TQ \to \mathbb{R} \times T^*Q$ the Legendre transformation for L given by $(t, q, \dot{q}) \mapsto (t, q, p := \partial L/\partial \dot{q})$. We assume that L is hyperregular, i.e. that $\mathbb{F}L$ is a diffeomorphism between $\mathbb{R} \times TQ$ and $\mathbb{R} \times T^*Q$. If L is hyperregular, one can work out the velocities $\dot{q} = \dot{q}(t, q, p)$ in terms of (t, q, p) and define the Hamiltonian function (the "total energy") $H : \mathbb{R} \times T^*Q \to \mathbb{R}$ as $H(t, q, p) = p^T \dot{q}(t, q, p) - L(t, q, \dot{q}(t, q, p))$, where the inverse of the Legendre transformation to express $\dot{q} = \dot{q}(t, q, p)$ has been used.

From the Lagrangian $L : \mathbb{R} \times TQ \to \mathbb{R}$ we can derive the Euler–Lagrange equations using a variational principle, as follows. Denote by $C^2(q_0, q_1)$ the set of twice differentiable curves with fixed end-points $q_0, q_1 \in Q$, that is, $C^2(q_0, q_1) = \{q : [0, T] \longrightarrow Q |\, q \text{ is } C^2, q(0) = q_0, q(T) = q_1\}$, and define the *action functional* $\mathcal{J} : C^2(q_0, q_1) \longrightarrow \mathbb{R}$, given by $q(\cdot) \mapsto \mathcal{J}(q(\cdot)) = \int_0^T L(t, q(t), \dot{q}(t))\, dt$. Critical points of this functional are described by the solutions of Euler–Lagrange equations, $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = 0$, that is,

$$\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}\ddot{q}^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j}\dot{q}^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial t} - \frac{\partial L}{\partial q^i} = 0. \tag{1}$$

Since L is hyperregular, the matrix $\mathrm{Hess}(L) := \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}\right)$ is non-singular. Hence, Eqs. (1) can be written as a system of explicit second-order time-dependent differential equations.

Two intrinsic geometrical objects (i.e., independent of the choice of local coordinates or the regularity of the Lagrangian), characterizing the tangent bundle TQ, are the Liouville vector field Δ and the vertical endomorphism S. These geometric objects allow, for instance, to describe the energy function of the system on the tangent bundle (instead of a Hamiltonian formalism on the cotangent bundle) and to describe the tangent bundle version of Noether theorem. Both can be regarded in a natural way as living on $\mathbb{R} \times TQ$ and we shall denote these extensions by the same symbols. In local coordinates, these geometrical objects can be written as $\Delta(q^i, v^i) = v^i \frac{\partial}{\partial \dot{q}^i}$ and $S(X^i \frac{\partial}{\partial q^i} + Y^i \frac{\partial}{\partial \dot{q}^i}) = X^i \frac{\partial}{\partial \dot{q}^i}$.

By using the Liouville vector field we define the energy function E_L on $\mathbb{R} \times TQ$ as $E_L = \Delta L - L$, or locally as $E_L = \dot{q}^i \frac{\partial L}{\partial \dot{q}^i} - L$. From Eqs. (1) it follows that the energy, in general, is not preserved in the non-autonomous case. In fact,

$$\frac{d}{dt}E_L = -\frac{\partial L}{\partial t}\,. \tag{2}$$

Remark 1. Alternatively, since L is hyperregular, one can construct the energy function $E_L : \mathbb{R} \times TQ \to \mathbb{R}$ by using the Legendre transformation $\mathbb{F}L : TQ \to T^*Q$ [19] as $E_L(t, q, \dot{q}) = \langle \mathbb{F}L(t, q, \dot{q}), \dot{q}\rangle - L(t, q, \dot{q})$.

Next, we define two lifts of vector fields on Q to TQ. Denote by $\mathfrak{X}(Q)$ the set of vector fields on Q and let $X^V \in \mathfrak{X}(Q)$ the *vertical lift* of $X \in \mathfrak{X}(Q)$, that is, the vector field on TQ given by

$$X^V(v_q) = \left.\frac{d}{dt}\right|_{t=0} (v_q + tX(q)) = (X(q))^V_{v_q}, \quad \forall v_q \in T_qQ.$$

Locally, $X^V = X^i \frac{\partial}{\partial \dot{q}^i}$ where $X = X^i \frac{\partial}{\partial q^i}$.

By denoting $\{\Phi_t^X\}$ the flow of a vector field $X \in \mathfrak{X}(Q)$, we can also define the *complete lift* $X^C \in \mathfrak{X}(TQ)$ of X in terms of its flow which is the tangent lift $\{T\Phi_t^X\}$. In other words, $X^C(v_q) = \left.\frac{d}{dt}\right|_{t=0} \left(T_q\Phi_t^X(v_q)\right)$. In coordinates, $X^C = X^i \frac{\partial}{\partial q^i} + \dot{q}^j \frac{\partial X^i}{\partial q^j} \frac{\partial}{\partial \dot{q}^i}$. As before, we denote by the same symbols the corresponding extensions to $\mathbb{R} \times TQ$. Therefore, $X^V(t, v_q) = (0_t, X^V(v_q))$ and $X^C(t, v_q) = (0_t, X^C(v_q))$.

Using the vertical and complete lifts the Euler–Lagrange equations can be alternatively described as follows [20,21]. A curve $q(t)$ is a solution of Euler–Lagrange equations for L if and only if

$$\frac{d}{dt}\left(X^V(L)(q(t), \dot{q}(t))\right) = X^C(L)(q(t), \dot{q}(t)), \quad \forall\, X \in \mathfrak{X}(Q). \tag{3}$$

In this paper we are only interested in symmetries that come from vector fields on Q. This motivates the following definitions.

Definition 2.1. A vector field $X \in \mathfrak{X}(Q)$ is said to be a **symmetry of the Lagrangian** $L : \mathbb{R} \times TQ \to \mathbb{R}$ if

$$X^C(L) = 0.$$

Denoting by $d_T f : \mathbb{R} \times TQ \to \mathbb{R}$ the differential of a function $f : \mathbb{R} \times Q \to \mathbb{R}$, that is, $d_T f = \frac{\partial f}{\partial t} + \dot{q}^i \frac{\partial f}{\partial q^i}$ we can define a more general class of symmetries called Noether symmetries.

Definition 2.2. A vector field $X \in \mathfrak{X}(Q)$ is said to be a **Noether symmetry** of $L : \mathbb{R} \times TQ \to \mathbb{R}$ if

$$X^C(L) = d_T f, \tag{4}$$

for some function $f \in C^\infty(\mathbb{R} \times Q)$.

Observe that symmetries of the Lagrangian are a particular type of Noether symmetries with $f = 0$ (or $f =$ constant, in general).

From the Euler–Lagrange equations (3), together with (4), it follows the celebrated Noether theorem for the relation between symmetries and first integrals.

Theorem 2.3 (*Noether Theorem*)**.** *If X is a Noether symmetry, that is $X^C(L) = d_T f$. Then, $X^V(L) - f$ is a constant of the motion for the Euler–Lagrange equations for L.*

Next, assume that G is a Lie group with Lie algebra $\mathfrak{g}$ and $\Phi : G \times Q \to Q$ a smooth left action of G on Q. The infinitesimal generator $\xi_Q \in \mathfrak{X}(Q)$ corresponding to an element $\xi \in \mathfrak{g}$ is defined by (see, for instance, [22] Section 2.8)

$$\xi_Q(q) = \left.\frac{d}{ds}\right|_{s=0} \Phi(\exp(s\xi), q). \tag{5}$$

Denote by $\{\Phi_s^{\xi_Q}\}$ the flow of ξ_Q then $\{T\Phi_s^{\xi_Q}\}$ is the flow of ξ_Q^C. The Lie group G is said to be a **Lie group of symmetries** for L if for all $\xi \in \mathfrak{g}$ and s, $L(t, T\Phi_s^{\xi_Q}(v_q)) = L(t, v_q)$. Infinitesimally, the previous condition is equivalent to

$$\xi_Q^C(L) = 0 \quad \text{for all} \quad \xi \in \mathfrak{g} \tag{6}$$

That is, if for any $\xi \in \mathfrak{g}$ we have that ξ_Q is a symmetry of the Lagrangian as in Definition 2.1.

As a consequence of Noether Theorem 2.3 we deduce that for all $\xi \in \mathfrak{g}$ we have that such that $\xi_Q^V(L)$ is a constant of the motion for the Euler–Lagrange equations for L.

Example 1. Consider the Lagrangian function $\mathbf{L} : T\mathbb{R}^n \equiv \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ given by

$$\mathbf{L}(q, \dot{q}) = \frac{1}{2}\|\dot{q}\|^2 - V(q), \tag{7}$$

$q = (q_1, \ldots, q_n) \in \mathbb{R}^n$ and $V : \mathbb{R}^n \to \mathbb{R}$ is a potential function which is assumed to be $SE(n)$-invariant [23].

Next, consider the non-autonomous Lagrangian $L : \mathbb{R} \times TQ \to \mathbb{R}$ given by $L(t, q, \dot{q}) = e^{-\kappa t}\mathbf{L}(q, \dot{q})$. The corresponding Euler–Lagrange equations for L are

$$\ddot{q}_i = \kappa \dot{q}_i - \nabla_{q_i} V. \tag{8}$$

In this case we have the energy of L and $\mathbf{L}$ are related by $E_L = e^{-\kappa t}E_{\mathbf{L}}$. Therefore using Eq. (2) it follows that $\frac{dE_L}{dt} = \kappa L$, indicating that the energy is not conserved along the evolution of the system. But, more interesting is to observe that $\frac{dE_{\mathbf{L}}}{dt} = \kappa\|\dot{q}\|^2$ and therefore we have dissipation of energy if $k < 0$, preservation if $k = 0$ and energy growth if $k > 0$.

The time-dependent Lagrangian L is $SE(n)$-invariant under the Lie group action $\Phi : SE(n) \times \mathbb{R}^n \to \mathbb{R}^n$ given by $\Phi(R, q) = \Phi(R, q_1, \ldots, q_n) = (Rq_1, Rq_2, \ldots, Rq_n)$ where $q_a \in \mathbb{R}$, $1 \le a \le n$. That is,

$$L(t, Rq_1, \ldots, Rq_n, R\dot{q}_1, \ldots, R\dot{q}_n) = L(t, q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n).$$

Infinitesimally this invariance means that $\xi_Q^C(L) = 0$ for any $\xi \in SE(d)$. Using that $\xi_Q^C(q)(L) = e^{-\kappa t}\xi_Q^C(q)(\mathbf{L})$, then $\xi_Q^C(\mathbf{L}) = 0$. Therefore, by Noether Theorem 2.3 it follows that $\xi_Q^V(L) = (e^{-\kappa t}\xi_Q^V(q)(\mathbf{L}))$ are constants of the motion for all $\xi \in \mathfrak{g}$ for the system given by Eqs. (8). As a consequence, if $k < 0$, we deduce the exponential decay of the functions $J_\xi := \xi_Q^V(q)(\mathbf{L})$:

$$\|J_\xi(q(t), \dot{q}(t))\| = e^{-\kappa t}\|J_\xi(q(0), \dot{q}(0))\|. \tag{9}$$

Note that in the case $d = 3$, we have two types of infinitesimal generators:

[(a)] Translation in the direction $\mathbf{a} \in \mathbb{R}^n$ makes the Lagrangian $SE(n)$-invariant. In this case, the infinitesimal generator is given by $\xi_Q = \mathbf{a} \cdot \frac{\partial}{\partial q}$. Therefore, by (9) the *linear momentum* $J_\xi = \xi_Q^V(q)(\mathbf{L}) = \mathbf{a} \cdot \dot{q}$ decays exponentially.

[(b)] Rotations in the system about some fixed axis makes the Lagrangian L also $SE(n)$-invariant. For instance, with $n = 3$, by considering rotations along the z-axis, the infinitesimal generator is given by the vector field $\xi_Q = \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$. In this case, by (9), the quantity which exponentially decays is the *angular momentum* $J_\xi = \xi_Q^V(q)(\mathbf{L}) = x\dot{y} - y\dot{x}$.

3. Symmetries and constants of the motion for discrete-time non-autonomous mechanical systems

Variational integrators (see [2] for details) are derived from a discrete variational principle. These integrators retain some of the main geometric properties of the continuous-time systems, such as symplecticity, momentum conservation (as long as the symmetry survives the discretization procedure), and good (bounded) behaviour of the energy associated to the system (see [3] and references therein).

A *discrete Lagrangian* is a differentiable function $L_d : Q \times Q \to \mathbb{R}$, which may be considered as an approximation of the action integral defined by a continuous regular Lagrangian $L : TQ \to \mathbb{R}$. That is, given a time step $h > 0$ small enough, $L_d(q_0, q_1) \approx \int_0^h L(q(t), \dot{q}(t))\, dt$, where $q(t)$ is the unique solution of the Euler–Lagrange equations for L with boundary conditions $q(0) = q_0$ and $q(h) = q_1$.

Construct the grid $\{t_k = kh \mid k = 0, \ldots, N\}$, with $Nh = T$ and define the discrete path space $\mathcal{C}_d := \{q_d : \{t_k\}_{k=0}^N \to Q\}$. We identify a discrete trajectory $q_d \in \mathcal{C}_d$ with its image $q_d = \{q_k\}_{k=0}^N$, where $q_k := q_d(t_k)$. Define

$$\mathcal{C}_d(q_0, q_N) = \left\{q_d : \{k\}_{k=0}^N \to Q \mid q_d(0) = q_0, q_d(N) = q_N\right\}.$$

The discrete action $\mathcal{A}_d : \mathcal{C}_d(q_0, q_N) \to \mathbb{R}$ for a sequence q_d is calculated by summing the discrete Lagrangian on each adjacent pair and is defined by

$$\mathcal{A}_d(q_d) = \mathcal{A}_d(q_0, \ldots, q_N) := \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}). \tag{10}$$

For any product manifold $Q_1 \times Q_2$, $T^*_{(q_1,q_2)}(Q_1 \times Q_2) \simeq T^*_{q_1}Q_1 \oplus T^*_{q_2}Q_2$, for $q_1 \in Q_1$ and $q_2 \in Q_2$ where T^*Q denotes the cotangent bundle of a differentiable manifold Q. Therefore, any covector $\alpha \in T^*_{(q_1,q_2)}(Q_1 \times Q_2)$ admits a unique decomposition $\alpha = \alpha_1 + \alpha_2$ where $\alpha_i \in T^*_{q_i}Q_i$, for $i = 1, 2$. Thus, given a discrete Lagrangian L_d we have the following decomposition $dL_d(q_0, q_1) = D_1L_d(q_0, q_1) + D_2L_d(q_0, q_1)$, where $D_1L_d(q_0, q_1) \in T^*_{q_0}Q$ and $D_2L_d(q_0, q_1) \in T^*_{q_1}Q$. Discrete Euler Lagrange equations (see [2] for instance) are given by a critical sequence for $\mathcal{A}_d$ on the space $\mathcal{C}_d(q_0, q_N)$. That is, the *discrete Euler–Lagrange equations* are

$$D_1L_d(q_{k+1}, q_{k+2}) + D_2L_d(q_k, q_{k+1}) = 0, \ \forall k = 0, \ldots, N-2,$$

where D_1 and D_2 denote the partial derivatives with respect to the first and second component of L_d, respectively.

For non-autonomous systems [10,13] we introduce, in the discrete setting, a family of maps $L_d^k : Q \times Q \to \mathbb{R}$, $k = 0, \ldots, N-1$ where we are now fixing the number of steps $N \in \mathbb{N}$ and considering a discrete Lagrangian on the set of discrete sequences defined on each step $q_d : \{k\}_{k=0}^N \to Q$.

The family of discrete Lagrangians $\{L_d^k\}_{k=0}^{N-1}$ will be called *discrete time-dependent Lagrangian* and simply denoted by L_d^k.

We look for the extremals of the corresponding discrete action given by $S_d(q_d) = \sum_{k=0}^{N-1} L_d^k(q_k, q_{k+1})$. The stationary condition for variations vanishing at the end points of the discrete sequences gives rise to the *discrete Euler–Lagrange equations* [13]

$$D_1L_d^{k+1}(q_{k+1}, q_{k+2}) + D_2L_d^k(q_k, q_{k+1}) = 0, \ k = 0, \ldots, N-2. \tag{11}$$

The discrete Euler–Lagrange equations implicitly defines a family of local discrete flows $\{\Psi_d^{k,k+1}\}_{k=0}^{N-2}$ as

$$\begin{array}{rccc} \Psi_d^{k,k+1} : & Q \times Q & \longrightarrow & Q \times Q \\ & (q_k, q_{k+1}) & \longmapsto & (q_{k+1}, q_{k+2}(q_k, q_{k+1}, k)) \end{array} \tag{12}$$

where q_{k+2} is locally well defined by using the discrete Euler–Lagrange equations and assuming the non-singularity of the matrix $D_{12}L_d^k(q_k, q_{k+1})$ for each k and $(q_k, q_{k+1}) \in Q \times Q$. Observe that the map $\Psi_d^{k,k+1}$ transforms a point (q_k, q_{k+1}) at a discrete time k to a new point (q_{k+1}, q_{k+2}) now at discrete time $k+1$.

Eqs. (11) define the integration scheme $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$. By defining the discrete (post and pre) momenta

$$\begin{aligned} p_k^+ &:= D_2L_d^{k-1}(q_{k-1}, q_k),\ k = 1, \ldots, N \\ p_k^- &:= -D_1L_d^k(q_k, q_{k+1}),\ k = 0, \ldots, N-1, \end{aligned} \tag{13}$$

Eqs. (11) lead to the integration scheme $(q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, by writing (11) as $p_k^- = p_k^+$.

Given a vector field $X \in \mathfrak{X}(Q)$ we can define the vector fields $X^{C,d}$ and $X^{V,d}$ in $X \in \mathfrak{X}(Q \times Q)$ by $X^{C,d}(q_0, q_1) = (X(q_0), X(q_1))$ and $X^{V,d}(q_0, q_1) = (X(q_0), 0_{q_1})$. In terms of these vector fields, the discrete Euler–Lagrange equations can be writen similarly to (3), as (see [21] for details)

$$X^{C,d}(q_k, q_{k+1})(L_d^k) = \left(X^{V,d}(q_k, q_{k+1})(L_d^k) - X^{V,d}(q_{k+1}, q_{k+2})(L_d^{k+1})\right), \tag{14}$$

$\forall X \in \mathfrak{X}(Q),\ k = 0, \ldots, N-2$.

Definition 3.1. A vector field $X \in \mathfrak{X}(Q)$ is said to be a **symmetry of the discrete time-dependent Lagrangian** $L_d^k : Q \times Q \to \mathbb{R}$ if for each $k \in \{0, \ldots, N-1\}$,

$$X^{C,d}(L_d^k) = 0.$$

For a family f of functions, $f^k : Q \to \mathbb{R}$, $k \in \{0, \ldots, N-1\}$, define $d_T^k f : Q \times Q \to \mathbb{R}$ by

$$d_T^k f(q_k, q_{k+1}) = f^{k+1}(q_{k+1}) - f^k(q_k).$$

Then, we can define Noether symmetries for the discrete-time Lagrangian L_d^k as follows.

Definition 3.2. A vector field $X \in \mathfrak{X}(Q)$ is said to be a **discrete Noether symmetry** of $L_d^k : Q \times Q \to \mathbb{R}$ if

$$X^{C,d}(L_d^k) = d_T^k f \tag{15}$$

for each $k \in \{0, \ldots, N-1\}$ and for a family f of functions $f^k : Q \to \mathbb{R}$.

In the same way as the continuous-time case, as a consequence of the discrete Euler–Lagrange equations (14), together with (15), we deduce Noether Theorem for the relation between symmetries of the discrete Lagrangian and first integrals of the discrete Euler–Lagrange equations.

Theorem 3.3 (*Discrete Noether Theorem*)**.** *If $X \in \mathfrak{X}(Q)$ is a discrete Noether symmetry for the discrete-time Lagrangian L_d^k, that is $X^{C,d}(L_d^k) = d_T^k f$, then, $X^{V,d}(L_d^k) - f^k$ is a constant of the motion for the discrete Euler–Lagrange equations for L_d^k for each k, $k = 0, \ldots, N-1$.*

As in Section 2, consider the action of a Lie group G on Q, $\Phi : G \times Q \to Q$, with infinitesimal generator as (5). This action can be lifted to $Q \times Q$ by $\Phi_g^{Q\times Q}(q_0, q_1) = (\Phi_g(q_0), \Phi_g(q_1))$ which has an infinitesimal generator $\xi_{Q\times Q} : Q \times Q \to T(Q \times Q)$ given by $\xi_{Q\times Q}(q_0, q_1) = (\xi_Q(q_0), \xi_Q(q_1)) = \xi_Q^{C,d}(q_0, q_1)$.

Assume that the family of discrete Lagrangians L_d^k is invariant under the lifted action, that is, for all $g \in G$

$$(L_d^k \circ \Phi_g^{Q\times Q})(q_0, q_1) = L_d^k(q_0, q_1),\ \ \forall (q_0, q_1) \in Q \times Q\ .$$

Infinitesimally, this is equivalent to

$$(\xi_{Q\times Q})^{C,d}(L_d^k) = 0,\ \text{for all } \xi \in \mathfrak{g}. \tag{16}$$

That is ξ_Q is symmetry of the discrete Lagrangian L_d^k.

From Eqs. (14) and (16) we obtain a discrete-time version of Noether Theorem as follows

Theorem 3.4. *Let G be a Lie group of symmetries for L_d^k, that is, $(\xi_{Q\times Q})^{C,d}(L_d^k) = 0$ for all k and $\xi \in \mathfrak{g}$. Then, $(\xi_{Q\times Q})^{V,d}(L_d^k)$ is a constant of the motion for the discrete Euler–Lagrange equations for L_d^k.*

Example 2. Consider the time-dependent Lagrangian function $L : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ given in Example 1 by

$$L(t, q, \dot{q}) = e^{-\kappa t}\left(\frac{1}{2}\|\dot{q}\|^2 - V(q)\right). \tag{17}$$

To construct the geometric integrator, the velocities are discretized by finite-differences, i.e., $\dot{q}_i \equiv \frac{q_{k+1}^i - q_k^i}{h}$ for $t \in [t_k, t_{k+1}]$. The discrete Lagrangian $L_{d,h}^k : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is given by setting the trapezoidal discretization for the

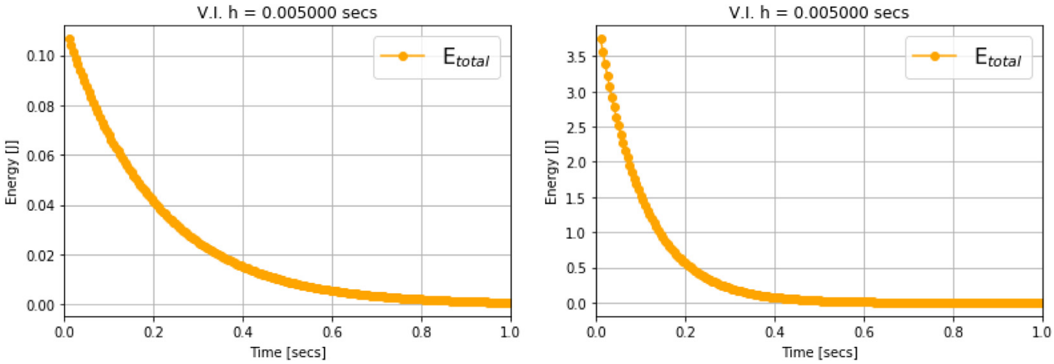

Fig. 1. Exponential decay for the rate of change of the total energy of system. The left figure shows the evolution of the non-autonomous energy function while the right figure corresponds with the evolution of the autonomous energy function.

time-dependent Lagrangian L given by (40), that is,

$$L^k_{d,h}(q_k, q_{k+1}) = \frac{h}{2}L\left(kh, q_k, \frac{q_{k+1}-q_k}{h}\right) + \frac{h}{2}L\left((k+1)h, q_{k+1}, \frac{q_{k+1}-q_k}{h}\right)$$

where, $h > 0$ is the time step.

The discrete Euler–Lagrange equations for $L^k_{d,h}$ are given by

$$\begin{aligned} 0 =& (q_{k+1}-q_k)e^{-\kappa(kh)} - (q_{k+2}-q_{k+1})e^{-\kappa h(k+2)} \\ &- e^{-\kappa h(k+1)}(q_k - 2q_{k+1} + q_{k+2} + h\nabla_{q_{k+1}}V(q_{k+1})). \end{aligned} \tag{18}$$

After some calculus we can write Eqs. (41) as the following explicit integration scheme

$$q_{k+2} = \hat{\kappa}_h q_{k+1} - \kappa_h q_k - h\bar{\kappa}_h \nabla_{q_{k+1}}V(q_{k+1}), \tag{19}$$

with $\kappa_h = \frac{e^{\kappa hk}+1}{e^{-\kappa hk}+1}$, $\bar{\kappa}_h = \frac{1}{e^{-\kappa hk}+1}$, $\hat{\kappa}_h = 1+\kappa_h = \frac{2+e^{-\kappa hk}+e^{\kappa hk}}{e^{-\kappa hk}+1}$.

Note that the previous equations are a set of $n(N-1)$ for the $n(N+1)$ unknowns $\{q_k\}_{k=0}^N$. Nevertheless the boundary conditions on initial positions and velocities $q_0 = q(0)$, $v_{q_0} = \dot{q}(0)$ contribute to $2n$ extra equations that convert Eqs. (41) into a nonlinear root finding problem of $n(N-1)$ equations and the same amount of unknowns. To start the algorithm we use the boundary conditions for the first two steps, that is, $q_0 = q(0)$ and $q_1 = hv_{q_0} + q_0 = h\dot{q}(0) + q(0)$.

The energy function is also discretized by using a trapezoidal discretization. In particular, the energy $E_L : \mathbb{R}\times TQ \to \mathbb{R}$ is given by

$$E_L(t, q, \dot{q}) = e^{-\kappa t}\left(\frac{1}{2}\|\dot{q}\|^2 + V(q)\right).$$

Using the trapezoidal rule for E_L, the discrete energy function $E_d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is given by

$$E_d(q_k, q_{k+1}) = \frac{1}{2h}\|q_{k+1}-q_k\|^2(e^{-\kappa kh} + e^{-\kappa(k+1)h}) + \frac{h}{2}(e^{-\kappa hk}V(q_k) + e^{-\kappa(k+1)h}V(q_{k+1})). \tag{20}$$

Next we show the performance of the proposed variational integrator in numerical simulations. For simplicity we consider $Q = \mathbb{R}^3$ and $V(q) = 0$. Initial positions were arbitrary selected as $q_0 = [18, 6, 10]$ and we set the initial velocities to be $v_0 = [2.22, -1.86, 3.48]$. Note that by using the fact that $\dot{E}_L = \kappa L = \kappa E_L$, for $\kappa < 0$ the energy of the system decays exponentially, so, for simulation results we choose as damping gain $\kappa = -5$. The simulation for the energy behaviour was conducted with an end time of 1 s and time steps of $h = 0.005$ s, which results in $N = 200$ iterations. In Fig. 1, we show the exponential decay for the rate of change of the total energy function of the system, in both case, for the non-autonomous energy function (left figure) and the autonomous energy function (right figure).

Observe also that the Lagrangian $L^k_{d,h}$ is $SE(d)$-invariant, therefore applying the discrete Noether Theorem 3.4, it follows that for all $\xi \in \mathfrak{se}(d)$,

$$\xi_Q^{V,d}(q_k, q_{k+1})(L^k_{d,h}) = \xi_Q^{V,d}(q_{k+1}, q_{k+2})(L^{k+1}_{d,h}), \tag{21}$$

for all $k = 0, \dots, N-1$ and where $\{q_k\}$ is a solution of the discrete Euler–Lagrange equations. Fig. 2 shows an application of Noether Theorem 3.4. In particular, Fig. 2 (left figure) shows the preservation of the constants of the motion associated from translation symmetry, that is,

$$-D_1L^k_{d,h}(q_k, q_{k+1}) = e^{-\kappa kh}\left((1+e^{-kh})\left(\frac{q_{k+1}-q_k}{h}\right) - \frac{h}{2}\nabla_{q_k}V(q_k)\right), \tag{22}$$

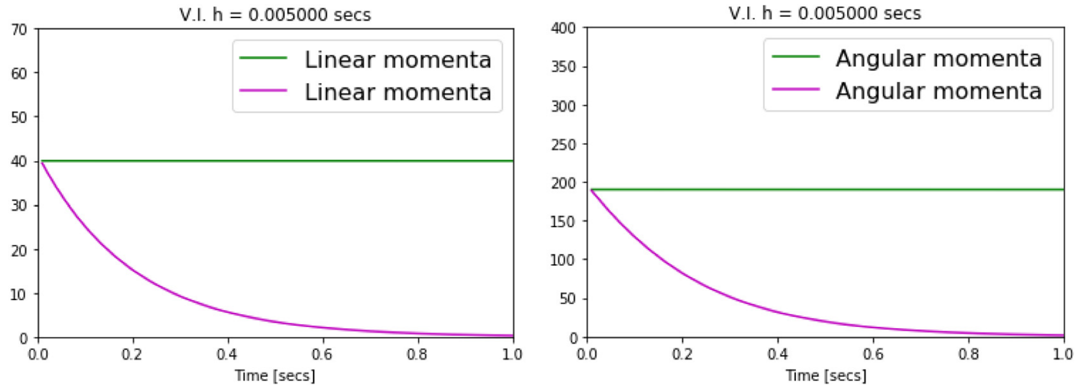

Fig. 2. Preservation of (22) (green-left) and exponential decay of the discretization of linear momentum (23) (purple-left). Preservation of (24) (green-right) and exponential decay of the discretization of angular momentum (25) (purple-right).

and the exponential decay of the corresponding discretization of linear momentum:

$$(1+e^{-kh})\left(\frac{q_{k+1}-q_k}{h}\right)-\frac{h}{2}\nabla_{q_k}V(q_k). \tag{23}$$

Similar simulation results can be obtained for the $SO(3)$-symmetry as is shown in Fig. 2 (right figure). Note that in the case of the associated constant of motion for $L^k_{d,h}$, it is given by

$$e^{-\kappa kh}\left((1+e^{-kh})\left(\frac{q_{k+1}-q_k}{h}\right)-\frac{h}{2}\nabla_{q_k}V(q_k)\right)\times q_{k+1}, \tag{24}$$

and the corresponding exponential decay of the discretization of the angular momentum is

$$\left((1+e^{-kh})\left(\frac{q_{k+1}-q_k}{h}\right)-\frac{h}{2}\nabla_{q_k}V(q_k)\right)\times q_{k+1}. \tag{25}$$

4. Discrete Hamiltonian flow for discrete-time non-autonomous mechanical systems

Consider $L : \mathbb{R}\times TQ \to \mathbb{R}$ as in Section 2. Since L is hyperregular we can determine the Hamiltonian function $H : \mathbb{R}\times T^*Q \to \mathbb{R}$ by using the Legendre transform $\mathbb{F}L : \mathbb{R}\times TQ \to \mathbb{R}\times T^*Q$ by

$$H = E_L\circ(\mathbb{F}L)^{-1} = p^T\dot{q}(t,q,p) - L(t,q,\dot{q}(t,q,p)),$$

which induces the cosymplectic structure (η, Ω_H) on $T^*Q\times\mathbb{R}$ with $\Omega_H = -d(\mathrm{pr}_1^*\theta_Q - H\eta) = \Omega_Q + dH\wedge \mathrm{d}t$ and $\eta = \mathrm{pr}_2^*\mathrm{d}t$, where pr_i, $i = 1, 2$, are the projections to each factor and θ_Q denotes the Liouville 1-form on T^*Q [19], given in induced coordinates by $\theta_Q = p_i\, dq^i$. We also denote by $\Omega_Q = -d\mathrm{pr}_1^*\theta_Q$ the pullback of the canonical symplectic 2-form $\omega_Q = -d\theta_Q$ on T^*Q. In coordinates, $\Omega_Q = dq^i\wedge dp_i$ but observe that now Ω_Q is presymplectic since $\ker\Omega_Q = \mathrm{span}\{\partial/\partial t\}$. Therefore in induced coordinates (t, q^i, p_i):

$$\Omega_H = dq^i\wedge dp_i + dH\wedge \mathrm{d}t\,, \qquad \eta = \mathrm{d}t.$$

We define the **evolution vector field** $E_H \in \mathfrak{X}(T^*Q\times\mathbb{R})$ by

$$i_{E_H}\Omega_H = 0\,, \qquad i_{E_H}\eta = 1 \tag{26}$$

In local coordinates the evolution vector field is:

$$E_H = \frac{\partial}{\partial t} + \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial}{\partial p_i}.$$

The integral curves of E_H are given by:

$$\dot{t} = 1\,, \qquad \dot{q}^i = \frac{\partial H}{\partial p_i}\,, \qquad \dot{p}_i = -\frac{\partial H}{\partial q^i}\,. \tag{27}$$

From Eq. (26) we deduce that the flow of E_H verifies the preservation relations

$$\mathcal{L}_{E_H}(\Omega_Q + dH\wedge \mathrm{d}t) = 0, \qquad \mathcal{L}_{E_H}\eta = 0. \tag{28}$$

The integral curves of E_H are precisely the curves of the form $t \mapsto \mathbb{F}L(\sigma'(t), t)$ where $\sigma : I \to Q$ is a solution of the Euler–Lagrange equations for the time-dependent Lagrangian $L : \mathbb{R}\times TQ \to \mathbb{R}$.

$$\begin{tikzcd}
& (q_k, q_{k+1}) \arrow[rr, mapsto, "\Psi_d^{k,k+1}"] \arrow[dl, mapsto, "\mathbb{F}^-_{L_d^{k+1}}"'] \arrow[dr, mapsto, "\mathbb{F}^+_{L_d^k}"] & & (q_{k+1}, q_{k+2}) \arrow[dl, mapsto, "\mathbb{F}^-_{L_d^{k+2}}"'] \arrow[dr, mapsto, "\mathbb{F}^+_{L_d^{k+1}}"] & \\
(q_k, p_k) \arrow[rr, mapsto, "\widetilde{\Psi}_d^{k,k+1}"'] & & (q_{k+1}, p_{k+1}) \arrow[rr, mapsto, "\widetilde{\Psi}_d^{k+1,k+2}"'] & & (q_{k+2}, p_{k+2})
\end{tikzcd}$$

Fig. 3. Correspondence between the discrete Lagrangian and the discrete Hamiltonian flows.

Denote by $\Psi_s : \mathcal{U} \subset T^*Q \times \mathbb{R} \to T^*Q \times \mathbb{R}$ the flow of the evolution vector field E_H, where $\mathcal{U}$ is an open subset of $T^*Q \times \mathbb{R}$. Observe that $\Psi_s(\alpha_q, t) = (\Psi_{t,s}(\alpha_q), t + s)$, $\alpha_q \in T_q^*Q$, where $\Psi_{t,s}(\alpha_q) = \mathrm{pr}_1(\Psi_s(\alpha_q, t))$. Therefore from the flow of E_H we induce a map

$$\Psi_{t,s} : \mathcal{U}_t \subseteq T^*Q \to T^*Q$$

where $\mathcal{U}_t = \{\alpha_q \in T^*Q \mid (\alpha_q, t) \in \mathcal{U}\}$. Observe that if we know $\Psi_{t,s}$ for all t, we can recover the flow Ψ_s of E_H.

From Eqs. (28) we have that $\Psi_s^*(\Omega_Q + dH \wedge \mathrm{d}t) = \Omega_Q + dH \wedge \mathrm{d}t$ and $\Psi_s^*(\eta) = \eta$. The previous preservation properties are associated with the symplecticity of the family of maps $\{\Psi_{t,s} : T^*Q \to T^*Q\}$. In particular, for all t, s with s small enough it has been show in [10] that $\Psi_{t,s} : \mathcal{U}_t \subseteq T^*Q \to T^*Q$ is a symplectomorphism, that is, $\Psi_{t,s}^*\omega_Q = \omega_Q$.

Given a discrete Lagrangian $L_d^k : Q \times Q \to \mathbb{R}$, the *discrete Legendre transformations* $\mathbb{F}^{\pm}_{L_d^k} : Q \times Q \to T^*Q$ are defined at each k through the momentum Eqs. (13) as

$$\mathbb{F}^+_{L_d^k}(q_0, q_1) =(q_1, D_2L_d^k(q_0, q_1)) = (q_1, p_1) \tag{29}$$

$$\mathbb{F}^-_{L_d^k}(q_0, q_1) =(q_0, -D_1L_d^k(q_0, q_1)) = (q_0, p_0). \tag{30}$$

If for each k both discrete Legendre transformations are locally diffeomorphisms for nearby q_0 and q_1, then we say that L_d^k is *regular*. Using $\mathbb{F}^{\pm}_{L_d^k}$, the discrete Euler–Lagrange equations (11) can be written as

$$\mathbb{F}^-_{L_d^{k+1}}(q_{k+1}, q_{k+2}) = \mathbb{F}^+_{L_d^k}(q_k, q_{k+1}).$$

Consider $\Psi_d^{k,k+1} : Q \times Q \to Q \times Q$ defined by (12). It will be useful to note that

$$\mathbb{F}^+_{L_d^k} = \mathbb{F}^-_{L_d^{k+1}} \circ \Psi_d^{k,k+1}. \tag{31}$$

Definition 4.1. We define the **discrete Hamiltonian flow** $\widetilde{\Psi}_d^{k,k+1} : T^*Q \to T^*Q$ as

$$\widetilde{\Psi}_d^{k,k+1} = \mathbb{F}^-_{L_d^{k+1}} \circ \Psi_d^{k,k+1} \circ \left(\mathbb{F}^-_{L_d^{k+1}}\right)^{-1}, \quad \widetilde{\Psi}_d^{k,k+1}(q_0, p_0) = (q_1, p_1). \tag{32}$$

Alternatively, it can also be defined as

$$\widetilde{\Psi}_d^{k,k+1} = \mathbb{F}^+_{L_d^k} \circ \Psi_d^{k,k+1} \circ \left(\mathbb{F}^+_{L_d^k}\right)^{-1}, \quad \widetilde{\Psi}_d^{k,k+1}(q_0, p_0) = (q_1, p_1). \tag{33}$$

In analogy with [2] we have the following results:

Proposition 1. *The diagram in Fig. 3 is commutative.*

Proof Proposition 1. The central triangle is (31). The parallelogram on the left-hand side is commutative by (32), so the triangle on the left is commutative. The triangle on the right is the same as the triangle on the left, with shifted indices. Then parallelogram on the right-hand side is commutative and therefore the triangle on the right-hand side. ◇

Corollary 1. *The following definitions of the discrete Hamiltonian flow are equivalent:* $\widetilde{\Psi}_d^{k,k+1} = \mathbb{F}^+_{L_d^k} \circ \Psi_d^{k,k+1} \circ (\mathbb{F}^+_{L_d^k})^{-1}$, $\widetilde{\Psi}_d^{k,k+1} = \mathbb{F}^-_{L_d^{k+1}} \circ \Psi_d^{k,k+1} \circ (\mathbb{F}^-_{L_d^{k+1}})^{-1}$, $\widetilde{\Psi}_d^{k,k+1} = \mathbb{F}^+_{L_d^k} \circ (\mathbb{F}^-_{L_d^{k+1}})^{-1}$.

In addition, for each k we have that $(\mathbb{F}^+L_d^k)^*\omega_Q = (\mathbb{F}^-L_d^k)^*\omega_Q$ (see [2,10]), so, for each k, the discrete Hamiltonian flow $\widetilde{\Psi}_d^{k,k+1}$ is a **symplectic transformation**, that is $(\widetilde{\Psi}_d^{k,k+1})^*\omega_Q = \omega_Q$. Moreover, given the map $\widetilde{\Psi}_d^{k,k+1}(q_k, p_k) = (q_{k+1}, p_{k+1})$, we have the map $(kh, q_k, p_k) = ((k+1)h, q_{k+1}, p_{k+1})$ on $\mathbb{R} \times T^*Q$ giving explicitly the information of the evolution of discrete time.

Example 3. Continuating with Examples 1 and 2, by using that

$$D_1L_{d,h}^k(q_k, q_{k+1}) = -\frac{q_{k+1}-q_k}{h}\left(e^{-\kappa kh} + e^{-\kappa(k+1)h}\right) - \frac{h}{2}e^{-\kappa kh}\nabla_{q_k}V(q_k),$$
$$D_2L_{d,h}^k(q_k, q_{k+1}) = \frac{q_{k+1}-q_k}{h}\left(e^{-\kappa kh} + e^{-\kappa(k+1)h}\right) - \frac{h}{2}e^{-\kappa(k+1)h}\nabla_{q_{k+1}}V(q_{k+1}),$$

we define the Legendre transformations as

$$\mathbb{F}^+_{L_d^k}(q_k, q_{k+1}) = \left(q_{k+1}, \frac{q_{k+1}-q_k}{h}\left(e^{-\kappa kh} + e^{-\kappa(k+1)h}\right) - \frac{h}{2}e^{-\kappa(k+1)h}\nabla_{q_{k+1}}V(q_{k+1})\right),$$
$$\mathbb{F}^-_{L_d^k}(q_k, q_{k+1}) = \left(q_k, \frac{q_{k+1}-q_k}{h}\left(e^{-\kappa kh} + e^{-\kappa(k+1)h}\right) + \frac{h}{2}e^{-\kappa kh}\nabla_{q_k}V(q_k)\right).$$

Using the last two expressions and $\Psi_d^{k,k+1}$ given by (42), it follows the construction of the Hamiltonian flow $\widetilde{\Psi}_d^{k,k+1}$ by Corollary 1.

5. Backward error analysis for discrete-time non-autonomous mechanical systems

Next we will show the discrete Hamiltonian flow $\widetilde{\Psi}_d^{k,k+1}$ defined in (32) has an asymptotically correct decay behaviour by studying the rate of decay of a truncated modified Hamiltonian function following the approach of *Backward Error Analysis* [3] (Chapter IX), [24] (Sec. 4) — see also [25,26] and reference therein.

Consider the ordinary differential equation

$$\frac{d}{dt}y(t) = X(y(t)), \tag{34}$$

with X a complete vector field on a manifold M and $y(t) \in M$. The flow map for X is denoted by $R_X : \mathbb{R} \times M \to M$. We use the notation $R_X(t, q)$ or simply $R_{X,t}(q)$. The flow $R_{X,t}$ may be expressed using a exponential map notation as $R_{X,t}(q) = \exp(tX)(q)$, where t is a parameter and $\exp : \mathfrak{X}(M) \to \mathrm{Diff}(M)$, with $\mathrm{Diff}(M)$ denoting the set of diffeomorphisms on M and $\mathfrak{X}(M)$ the set of vector fields on M. In the following, we assume that the flow $\exp(tX)$ is not explicitly integrable, and therefore one may use a numerical method to simulate the flow. Under this assumption, a numerical approximation to the solution of (34) can be given by constructing a family of diffeomorphisms $\{\Phi_h\}_{h\geq 0}$ and then, for each h fixed, it may be possible to obtain the sequence $\{q_{h,n}\}_{n\in\mathbb{N}}$ satisfying $\Phi_h(q_{h,n}) = q_{h,n+1}$, called a numerical integrator. A **numerical integrator** for X is a family of one-parameter diffeomorphisms $\Phi_h : M \to M$ (smooth in h) satisfying $\Phi_0(x) = x$ with $x \in M$, and $\Phi_h(x) - \exp(hX)(x) = \mathcal{O}(h^{p+1})$ with $p \geq 1$ being the order of the integrator. Let us consider now the special case when $M = T^*Q$ (as in this paper). We recall that an integrator Φ_h is **symplectic** if it is a symplectic diffeomorphism with respect to the symplectic canonical structure ω_Q on T^*Q for each $h > 0$.

Consider the Hamilton equations (27) for $H : \mathbb{R} \times T^*Q \to \mathbb{R}$, that is the integral curves of the evolution vector field

$$E_H = \frac{\partial}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p} \tag{35}$$

We aim to study backward error analysis for $\widetilde{\Psi}_d^{k,k+1} : T^*Q \to T^*Q$, the discrete Hamiltonian flow defined in Definition 4.1 for the non-autonomous Hamiltonian system (27) at each fixed $t \in \mathbb{R}$ - recall that $\Psi_{t,s} : \mathcal{U}_t \subseteq T^*Q \to T^*Q$ is a symplectomorphism, in particular for $s = h$.

Using the extended Hamiltonian $H^{ext} : T^*(\mathbb{R} \times Q) \to \mathbb{R}$ defined by

$$H^{ext}(t, q, \mu, p) = \mu + H(t, q, p),$$

the corresponding equations of motion for the Hamiltonian vector field $X_{H^{ext}}$ are

$$\dot{q} = \frac{\partial H^{ext}}{\partial p} = \frac{\partial H}{\partial p},$$
$$\dot{p} = -\frac{\partial H^{ext}}{\partial q} = -\frac{\partial H}{\partial q},$$
$$\dot{t} = \frac{\partial H^{ext}}{\partial \mu} = 1,$$
$$\dot{\mu} = -\frac{\partial H^{ext}}{\partial t} = -\frac{\partial H}{\partial t}.$$

The Hamiltonian $X_{H^{ext}}$ projects onto E_H and therefore also their flows are related by the projection $pr : T^*(\mathbb{R}\times Q) \to \mathbb{R}\times T^*Q$ given by $pr(t,q,\mu,p) = (t,q,p)$.

Now we will see how to naturally extend the flow $\widetilde{\Psi}_d^{k,k+1} : T^*Q \to T^*Q$ to a symplectic discrete flow $\widetilde{\Psi}_h^{ext} : T^*(\mathbb{R}\times Q) \to T^*(\mathbb{R}\times Q)$. Consider the extended discrete Lagrangian $L_d^{ext} : Q\times Q\times\mathbb{R}\times\mathbb{R} \to \mathbb{R}$ subjected to the constraint $t_{k+1} = t_k + h$ and $t_0 = 0$ then

$$L_d^{ext}(q_k, q_{k+1}, t_k, t_{k+1}) = L_d^k(q_k, q_{k+1}),$$

for $t_k = kh$ and $t_{k+1} = h(k+1)$. Applying discrete variational calculus subjected to constraints we obtain the following implicit symplectic method (see [2,21,27])

$$\begin{aligned}
p_k &= -D_1 L_d^{ext}(q_k, q_{k+1}, t_k, t_{k+1}) = -D_1 L_d^k(q_k, q_{k+1}),\\
p_{k+1} &= D_2 L_d^{ext}(q_k, q_{k+1}, t_k, t_{k+1}) = D_2 L_d^k(q_k, q_{k+1}),\\
\mu_k &= -D_3 L_d^{ext}(q_k, q_{k+1}, t_k, t_{k+1}) + \lambda_k,\\
\mu_{k+1} &= D_4 L_d^{ext}(q_k, q_{k+1}, t_k, t_{k+1}) + \lambda_k,\\
t_{k+1} &= t_k + h,
\end{aligned}$$

where λ_k is a Lagrange multiplier associated to the constraint $t_{k+1} = t_k + h$. These equations implicitly define a symplectic flow $\widetilde{\Psi}_h^{ext} : T^*(\mathbb{R}\times Q) \to T^*(\mathbb{R}\times Q)$ by

$$\widetilde{\Psi}_h^{ext}(t_k, q_k, \mu_k, p_k) = (t_k + h, q_{k+1}, \mu_{k+1}, p_{k+1}).$$

Moreover $\widetilde{\Psi}_h^{ext}$ it is a numerical integrator for $X_{H^{ext}}$

Applying classical results of backward error analysis [3,24] we can derive a modified Hamiltonian vector field $\bar{X}_{H^{ext}}$ that can be written as an asymptotic expansion in terms of the step-size $h > 0$ as

$$\bar{X}_{H^{ext}} = \sum_{r=0}^{\infty} h^r X_r, \tag{36}$$

where each X_r is a real analytic vector field on $T^*(\mathbb{R}\times Q)$ and it may be determined by the integrator $\widetilde{\Psi}_h^{ext}$ as

$$X_r(t,q,\mu,p) = \lim_{h\to 0} \frac{\widetilde{\Psi}_h^{ext}(t,q,\mu,p) - \exp(hX_{h,r-1})(t,q,\mu,p)}{h^r}, \tag{37}$$

with $X_0 = X_{H^{ext}}$ and $X_{h,r} := \sum_{j=0}^{r} h^j X_j$.

Since the discretization $\widetilde{\Psi}_h^{ext}$ is symplectic there exist functions $H_r^{ext} : T^*(\mathbb{R}\times Q) \to \mathbb{R}$ such that each $X_r = X_{H_r^{ext}}$ with $X_0 = X_{H^{ext}}$ [3]. That is, the modified vector field $\bar{X}_{H^{ext}}$ associated to $\widetilde{\Psi}_h^{ext}$ is Hamiltonian $\bar{H}_{ext} : T^*(\mathbb{R}\times Q) \to \mathbb{R}$ with Hamiltonian function with formal expansion

$$\bar{H}_{ext} = H_{ext} + \sum_{r=1}^{\infty} h^r H_r^{ext}.$$

Furthermore, because the equation of motion in the variable t is integrated exactly (that is, $t_{k+1} = t_k + h$) we have that $\bar{H}_{ext}(q,t,p,\mu) = \mu + \bar{H}(q,p,t)$ and, in consequence, also $H_r^{ext} : \mathbb{R}\times T^*Q \to \mathbb{R}$. We can consider the truncated Hamiltonians: $\bar{H}_{ext}^N = H_{ext} + \sum_{r=1}^{N} h^r H_r^{ext}$. Therefore we have a truncated Hamiltonian $\bar{H}^N = H + \sum_{r=1}^{N} h^r H_r^{ext}$ on $\mathbb{R}\times T^*Q$. We have corresponding **evolution vector field** $E_{\bar{H}^N} \in \mathfrak{X}(T^*Q\times\mathbb{R})$ determined by

$$i_{E_{\bar{H}^N}} \Omega_{\bar{H}^N} = 0\,, \qquad i_{E_{\bar{H}^N}} \eta = 1 \tag{38}$$

As a consequence its flow preserves the 2-form $\Omega_{\bar{H}^N}$ and the 1-form η, being two important properties of this type of geometric integrators. In local coordinates the evolution vector field is given by

$$E_{\bar{H}^N} = \frac{\partial}{\partial t} + \frac{\partial \bar{H}^N}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial \bar{H}^N}{\partial q^i}\frac{\partial}{\partial p_i}.$$

As in Section 4 from the flow of $E_{\bar{H}^N}$ we induce the two-parameter symplectic family of maps $\Psi_{t,s}^{E_{\bar{H}^N}} : T^*Q \to T^*Q$.

From our previous considerations we deduce that $\widetilde{\Psi}_d^{k,k+1}(q,p) - \Psi_{kh,h}^{E_{\bar{H}^N}}(q,p) = \mathcal{O}(h^{N+1})$. In particular one has the following result for autonomous systems from [24] adapted to our non-autonomous context.

Lemma 5.1 (*Adapted from A. C. Hansen (2011) Theorem 4.1 [24]*)**.** *Let T^*Q be a real and analytic smooth manifold, d a Riemannian distance on T^*Q, a real analytic evolution vector field $E_{\bar{H}^N}$ on T^*Q and $\widetilde{\Psi}_d^{k,k+1}$ be a numerical integrator deduced from a family of discrete Lagrangians $\{L_d^k\}$ such that the induced symplectic method $\widetilde{\Psi}_d^{k,k+1} : T^*Q \to T^*Q$ is of order p such that it is analytical and $(q,p) \in \mathcal{K} \subset T^*Q$ with $\mathcal{K}$ compact. For each time step k there exists $\tau \in \mathbb{Z}$ depending on h and positive constants C, α, γ such that for $\Psi_{t,s}^{E_{\bar{H}^\tau}} : T^*Q \to T^*Q$ such that $d\left(\widetilde{\Psi}_d^{k,k+1}(q,p), \Psi_{kh,h}^{E_{\bar{H}^N}}(q,p)\right) \le Che^{-\gamma/h}$ for all $(q,p) \in \mathcal{K}$ and $h \le \alpha$, where $\widetilde{\Psi}_d^{k,k+1}$ must be considered as $\widetilde{\Psi}_d^{k,k+1} := \varphi \circ \widetilde{\Psi}_d^{k,k+1} \circ \varphi^{-1}$ for a given local chart (U,φ) on T^*Q.*

Finally, consider the truncated Hamiltonian $\bar{H}^N_{ext} = H_{ext} + \sum_{r=p}^{N} h^r H_r^{ext}$. Following [3], Section IX.8 we obtain the following result:

Theorem 5.2. *Assume that the Hamiltonian function $H_{ext} : \mathcal{U} \subset T^*(\mathbb{R} \times Q) \to \mathbb{R}$ where $\mathcal{U}$ is an open subset, and apply the symplectic method $\widetilde{\Psi}_h^{ext}$. If the numerical solution stays in a compact set $\mathcal{K} \subset \mathcal{U}$, then there exist h_0 and $N = N(h)$, (N equal to the largest integer satisfying $hN \leq h_0$) such that*

$$\bar{H}^N_{ext}(q_k, t_k, p_k, \mu_k) = \bar{H}^N_{ext}(q_0, t_0, p_0, \mu_0) + \mathcal{O}(e^{-h_0/2h}),$$
$$H_{ext}(q_k, t_k, p_k, \mu_k) = H_{ext}(q_0, t_0, p_0, \mu_0) + \mathcal{O}(h^p),$$

over exponentially long time intervals $nh \leq e^{h_0/2h}$.

6. Examples

6.1. Formation control of double integrator agents

Formation control of agents with double integrator dynamics can be seen as a stabilization system whose evolution can be described by a time-dependent Lagrangian function. Next we employ the previous constructions on variational integrators for time-dependent Lagrangian systems in the context of distance-based formation control algorithms.

6.1.1. Double integrator formation stabilization systems

Consider dimension $n \geq 2$ autonomous agents and denote by $\mathcal{N}$ the set of agents ($|\mathcal{N}|$ the total number of agents). Agent's evolve under a double integrator dynamics. We wish the agents reach a desired formation shape. To do that one needs to look for a minima of the potential function

$$V(q^{[1]}, \dots, q^{[|\mathcal{N}|]}) := \frac{1}{2}\sum_{a=1}^{|\mathcal{N}|}\sum_{b\in\mathcal{N}_a} V_{ab}(q^{[a]}, q^{[b]})$$

with

$$V_{ab}(q^{[a]}, q^{[b]}) := \frac{1}{4}(\|q^{[a]} - q^{[b]}\|^2 - d_{ab}^2)^2.$$

Here $q^{[a]} \in \mathbb{R}^d$ describes the position of an agent "a" in $\mathbb{R}^d$ ($d = 2$ or $d = 3$) with the neighbour set of agents $b \in \mathcal{N}_a \subset \{1, \dots, a-1, a+1, \dots, |\mathcal{N}|\}$ and given constants $d_{ab} > 0$ that define the desired distances of agents "a" and "b" for $a = 1, \dots, |\mathcal{N}|$, $b \in \mathcal{N}_a$. For any $\kappa > 0$ the second order system

$$\ddot{q} = -\kappa\dot{q} - \nabla V(q) \text{ with } q = (q^{[1]}, \dots, q^{[|\mathcal{N}|]}) \in \mathbb{R}^{d|\mathcal{N}|}, \tag{39}$$

called double integrator formation stabilization system [28], has decreasing energy $E = \|\dot{q}\|^2/2 + V(q)$ until a stationary point of $V(q)$ is reached since $\dot{E} = \dot{q}^T\ddot{q} + \dot{q}^T\nabla V = -\kappa\|\dot{q}\|^2 < 0$.

Note that the double integrator formation stabilization system (39) can be given by the Euler–Lagrange equations for the time-dependent Lagrangian function $L : \mathbb{R} \times T\mathbb{R}^{d|\mathcal{N}|} \to \mathbb{R}$ given by

$$L(t, q, \dot{q}) = e^{\kappa t}\left(\frac{1}{2}\sum_{a=1}^{|\mathcal{N}|}\|\dot{q}^{[a]}\|^2 - V(q)\right). \tag{40}$$

6.1.2. Derivation of the discretized equations of motion

To construct the geometric integrator, the velocities for each agent $a \in \mathcal{N}$ are discretized by finite-differences, i.e., $\dot{q}^{[a]} \approx \frac{q_{k+1}^{[a]} - q_k^{[a]}}{h}$ for $t \in [t_k, t_{k+1}]$. Denote also by $q_k = ((q_k^{[1]}), \dots, (q_k^{[|\mathcal{N}|]})) \in \mathbb{R}^{d|\mathcal{N}|}$. The discrete Lagrangian $L_{d,h}^k : \mathbb{R}^{d|\mathcal{N}|} \times \mathbb{R}^{d|\mathcal{N}|} \to \mathbb{R}$ is given by setting the trapezoidal discretization for the time-dependent Lagrangian L given by (40), that is,

$$L_{d,h}^k(q_k, q_{k+1}) = \frac{h}{2}L\left(kh, q_k, \frac{q_{k+1} - q_k}{h}\right) + \frac{h}{2}L\left((k+1)h, q_{k+1}, \frac{q_{k+1} - q_k}{h}\right)$$

where, $h > 0$ is the time step.

The discrete Euler–Lagrange equations for $L_{d,h}^k$ are given by

$$\begin{aligned} 0 =&(q_{k+1}^{[a]} - q_k^{[a]})e^{\kappa(kh)} - (q_{k+2}^{[a]} - q_{k+1}^{[a]})e^{\kappa h(k+2)} \\ &- e^{\kappa h(k+1)}(q_k^{[a]} - 2q_{k+1}^{[a]} + q_{k+2}^{[a]} + 2h^2\nabla_{q_{k+1}^{[a]}} V_{ab}^d(q_{k+1}^{[a]}, q_{k+1}^{[b]})), \end{aligned} \tag{41}$$

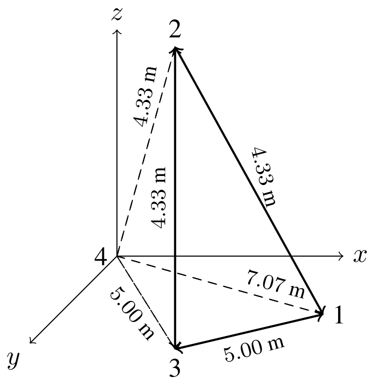

Fig. 4. Infinitesimal and minimal rigid graph considered in the numerical simulations.

for each $a \in \mathcal{N}$ and $b \in \mathcal{N}_a$, where we have used that

$$V^d_{ab} = \frac{1}{2}\sum_{b\in\mathcal{N}_a}(V^d_{ab}(q^{[a]}_k, q^{[b]}_k) + V^d_{ab}(q^{[a]}_{k+1}, q^{[b]}_{k+1})),$$

that is, V^d_{ab} is the trapezoidal discretization of V_{ab}.

After some calculus we can write Eqs. (41) as the following explicit integration scheme

$$q^{[a]}_{k+2} = \hat{\kappa}_h q^{[a]}_{k+1} - \kappa_h q^{[a]}_k - \bar{\kappa}_h \nabla_{q^{[a]}_{k+1}} V^d_{ab}(q^{[a]}_{k+1}, q^{[b]}_{k+1}), \tag{42}$$

for each $a \in \mathcal{N}$ and $b \in \mathcal{N}_a$, with $\kappa_h = \frac{1+e^{-\kappa h}}{1+e^{\kappa h}}$, $\bar{\kappa}_h = \frac{2h^2}{1+e^{\kappa h}}$, $\hat{\kappa}_h = 1 + \kappa_h = \frac{2+e^{\kappa h}+e^{-\kappa h}}{1+e^{\kappa h}}$, that is, for each $a \in \mathcal{N}$

$$\begin{cases} q^{[a]}_{k+2} &= \hat{\kappa}_h q^{[a]}_{k+1} - \kappa q^{[a]}_k - \bar{\kappa}_h \sum_{b\in\mathcal{N}_a} \Gamma^k_{ab}(q^{[a]}_{k+1} - q^{[b]}_{k+1}), \\ \Gamma^k_{ab} &= \|q^{[a]}_{k+1} - q^{[b]}_{k+1}\|^2 - d^2_{ab}. \end{cases}$$

Note that the previous equations are a set of $d|\mathcal{N}|(N-1)$ equations, $k = 0, \dots, N$ for the $d|\mathcal{N}|(N+1)$ unknowns $\{q^{[a]}_k\}^N_{k=0}$, with $1 \le a \le n = |\mathcal{N}|$. Nevertheless the boundary conditions on initial positions and velocities of the agents $q^{[a]}_0 = q_a(0)$, $v^{[a]}_{q_0} = \dot{q}_a(0)$ contribute to $2dn$ extra equations that convert Eqs. (41) in a nonlinear root finding problem of $dn(N-1)$ equations and the same amount of unknowns. To start the algorithm we use the boundary conditions for the first two steps, that is, $q^{[a]}_0 = q^{[a]}(0)$ and $q^{[a]}_1 = hv^{[a]}_{q_0} + q^{[a]}_0 = h\dot{q}_{[a]}(0) + q_{[a]}(0)$.

Remark 2. Observe also that the Lagrangian $L^k_{d,h}$ is $SE(d)$-invariant, since the inter-agent potential is $SE(d)$-invariant, therefore we can apply the discrete Noether Theorem 3.4. Both the linear and angular momentum in double-integrator formation systems are related with steering controller design for coordinating a formation as a whole at the steady state by using the linear and angular momentum of the centroid and therefore the variational integrators developed in this work could be used as for the steering control to achieve a desired formation.

6.1.3. Simulation results

Next, for simulation purposes we will restrict ourselves to the case $|\mathcal{N}| = 4$, $d = 3$, where the desired formation shape is depicted in Fig. 4 with neighbour relationships given by $\mathcal{N}_1 = \{2, 3, 4\}$, $\mathcal{N}_2 = \{1, 3, 4\}$, $\mathcal{N}_3 = \{1, 2, 4\}$ and $\mathcal{N}_4 = \{1, 2, 3\}$.

The explicit integration scheme (42) is given by

$$\begin{cases} q^{[1]}_{k+2} = & G^1_k - \bar{\kappa}_h \left(\Gamma^{k+1}_{12}(q^{[1]}_{k+1} - q^{[2]}_{k+1}) + \Gamma^{k+1}_{13}(q^{[1]}_{k+1} - q^{[3]}_{k+1}) + \Gamma^{k+1}_{14}(q^{[1]}_{k+1} - q^{[4]}_{k+1})\right) \\ q^{[2]}_{k+2} & G^2_k - \bar{\kappa}_h \left(\Gamma^{k+1}_{21}(q^{[2]}_{k+1} - q^{[1]}_{k+1}) + \Gamma^{k+1}_{23}(q^{[2]}_{k+1} - q^{[3]}_{k+1}) + \Gamma^{k+1}_{24}(q^{[2]}_{k+1} - q^{[4]}_{k+1})\right) \\ q^{[3]}_{k+2} = & G^3_k - \bar{\kappa}_h \left(\Gamma^{k+1}_{31}(q^{[3]}_{k+1} - q^{[1]}_{k+1}) + \Gamma^{k+1}_{32}(q^{[3]}_{k+1} - q^{[2]}_{k+1}) + \Gamma^{k+1}_{34}(q^{[3]}_{k+1} - q^{[4]}_{k+1})\right) \\ q^{[4]}_{k+2} = & G^4_k - \bar{\kappa}_h \left(\Gamma^{k+1}_{41}(q^{[4]}_{k+1} - q^{[1]}_{k+1}) + \Gamma^{k+1}_{42}(q^{[4]}_{k+1} - q^{[2]}_{k+1}) + \Gamma^{k+1}_{43}(q^{[4]}_{k+1} - q^{[3]}_{k+1})\right) \end{cases} \tag{43}$$

where $G^a_k = G(q^{[a]}_k, q^{[a]}_{k+1}) = \hat{\kappa}_h q^{[a]}_{k+1} - \kappa_h q^{[a]}_k$, $q^{[a]}_k = (x^a_k, y^a_k, z^a_k) \in \mathbb{R}^3$, $i = 1, \dots, 4$.

Initial positions were $q_0 = [1, 0, 0, 1, 0, 1, 0, -3, 0, 1, 0, -3]$ and we set the initial velocities to zero and damping gains $\kappa = 13$. In this case, an end time was settled of 2 s in steps of $h = 0.005$ s, resulting in $N = 400$ iterations. In Fig. 5

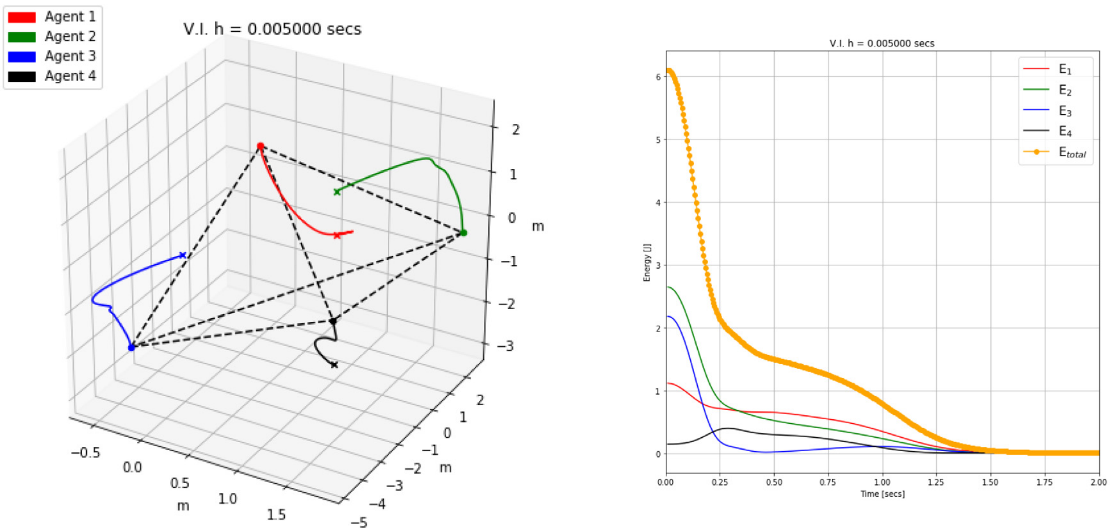

Fig. 5. Convergence of agents' trajectories by employing the variational integrator (left) and evolution of the discrete energy function in the 3-dimensional formation with pyramidal shape (right). The crosses denote the initial positions.

on the left we show the convergence of agents' trajectories by employing the variational integrator and in Fig. 5 on the right we shows the decrease of the energy, both per agent and total.

The energy function was discretized using a trapezoidal discretization. In particular, the total energy of each agent $E_a : T\mathbb{R}^{12} \to \mathbb{R}$ is given by

$$E_a(q^{[a]}, \dot{q}^{[a]}) = \frac{1}{2}\|\dot{q}^{[a]}\|^2 + \frac{1}{2}\sum_{b\in\mathcal{N}_b} V_{ab}(q^{[a]}, q^{[b]}).$$

Using the trapezoidal rule for E_a, the discrete energy function for each agent $E_a^d : \mathbb{R}^4 \times \mathbb{R}^4 \to \mathbb{R}$ is given by

$$E_a^d(q_k^{[a]}, q_{k+1}^{[a]}) = \frac{1}{2h^2}(q_{k+1}^{[a]} - q_k^{[a]})^2 + \frac{1}{4}\sum_{b\in\mathcal{N}_a}(V_{ab}^d(q_k^{[a]}, q_k^{[b]}) + V_{ab}^d(q_{k+1}^{[a]}, q_{k+1}^{[b]})). \tag{44}$$

6.2. Numerical integration in celestial mechanics

In several problems in celestial mechanics it is interesting to study the dynamics of the following second-order differential equation:

$$\ddot{q} + f(t)\dot{q} = -\nabla V(q) \tag{45}$$

An example is the Lane–Emden equation, used in modelling of stellar structures

$$\ddot{q} + \frac{2\dot{q}}{t} = -q^m$$

with $V(q) = \frac{q^{m+1}}{m+1}$.

We can write Eq. (45) as a time-dependent Lagrangian system by using the Lagrangian function

$$L(t, q, \dot{q}) = e^{\int f(t)dt}(\frac{1}{2}\|\dot{q}\|^2 - V(q)),$$

and apply our study of symmetries, constant of the motion and the construction of variational integrators for this time-dependent Lagrangian system.

For instance, in [16] the authors study a perturbed Kepler problem with linear drag that also depends on time:

$$\ddot{q} + \alpha\sin(\Omega t)\dot{q} + \gamma\frac{q}{|q|^3} = 0 \tag{46}$$

with $\alpha, \Omega, \gamma \in \mathbb{R}$. The authors use the contact formalism with Hamiltonian

$$\mathcal{H}(t, q, p, s) = \frac{|p|^2}{2} - \frac{\gamma}{|q|} + \alpha\sin(\Omega t)s$$

where s is an extra variable. Using the contact formalism they deduce the equations

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} = p, \tag{47}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q} - \frac{\partial \mathcal{H}}{\partial s} p = -\gamma \frac{q}{|q|^3} - \alpha \sin(\Omega t) p, \tag{48}$$

$$\dot{s} = \frac{\partial \mathcal{H}}{\partial p} p - \mathcal{H} = \frac{|p|^2}{2} + \frac{\gamma}{|q|} + \alpha \sin(\Omega t) s. \tag{49}$$

Observe that Eqs. (47) and (48) imply the modified Kepler equations (46). Using our formalism these equations are directly derived using the time-dependent Lagrangian

$$L(t, q, \dot{q}) = e^{-\frac{\alpha}{\Omega}\cos(\Omega t)} \left(\frac{|\dot{q}|^2}{2} + \frac{\gamma}{|q|} \right).$$

and we can directly apply Noether theorems and all the discrete variational methods developed in our paper.

7. Conclusions

We have constructed variational integrators for non-autonomous Lagrangian systems with fixed time step. In particular, a variational integrator for a time-dependent Lagrangian system was derived via a family of discrete Lagrangian functions each one for a fixed time step. This allows recovering at each step on the set of discrete sequences the preservation properties of variational integrators for autonomous Lagrangian systems such as symplecticity of the integrator or exponential decay of the energy due to backward error analysis. By assuming a regularity condition we can derive the corresponding discrete Hamiltonian flow. A Noether theorem for this class of systems was also obtained giving rise to a relation between Noether symmetries and constants of the motion for both the continuous-time and the discrete-time Euler–Lagrange equations. In further work we would like to study the applicability of backward error analysis in the Lagrangian side as in [29] but in the non-autonomous case and compare with the results obtained in this paper as well as comparisons with other integrators with fixed step-size, as for instance, the exponential Euler integrator [30]. We expect the proposed methods to have a better qualitative behaviour and stability properties due to their inherent geometric preservation construction (symmetry, symplecticity on fibres...) than other methods, especially in formation control of multi-agent systems with large $\mathcal{N}$. Another perspective is the extension to time-dependent forced and nonholonomic systems.

Data availability

No data was used for the research described in the article.

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