Discrete variational principles and Hamilton-Jacobi theory for mechanical systems and optimal control problems. *

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Abstract

In this paper we present a general framework that allows one to study discretization of certain dynamical systems. This generalizes earlier work on discretization of Lagrangian and Hamiltonian systems on tangent bundles and cotangent bundles respectively. In particular we show how to obtain a large class of discrete algorithms using this geometric approach. We give new geometric insight into the Newmark model for example and we give a direct discrete formulation of the Hamilton-Jacobi method. Moreover we extend these ideas to deriving a discrete version of the maximum principle for smooth optimal control problems.

We define discrete variational principles that are the discrete counterpart of known variational principles. For dynamical systems, we introduce principles of critical action on both the tangent bundle and the cotangent bundle. These two principles are equivalent and allow one to recover most of the classical symplectic algorithms. In addition, we prove that by increasing the dimensionality of the dynamical system (with time playing the role of a generalized coordinate), we are able to add conservation of energy to any (symplectic) algorithms derived within this framework. We also identify a class of coordinate transformations that leave the variational principles presented in this paper invariant and develop a discrete Hamilton-Jacobi theory. This theory allows us to show that the energy error in the (symplectic) integration of a dynamical system is invariant under discrete canonical transformations. Finally, for optimal control problems we develop a discrete maximum principle that yields discrete necessary conditions for optimality. These conditions are in agreement with the usual conditions obtained from Pontryagin maximum principle. We illustrate our approach with an example of a sub-Riemannian optimal control problem as well as simulations that motivate the use of symplectic integrators to compute the generating functions for the phase flow canonical transformation.

Key words: Variational integrators, Dynamical systems, Discrete optimal control
1 Introduction

Standard methods (called numerical integrators) for simulating motion take an initial condition and move objects in the direction specified by the differential equations. These methods do not directly satisfy the physical conservation laws associated with the system. An alternative approach to integration, the theory of geometric integrators[27,7], has been developed over the last two decades. These integrators strictly obey some of these physical laws, and take their name from the law they preserve. For instance, the class of energy-momentum integrators conserves energy and momenta associated with ignorable coordinates. Another class of geometric integrators is the class of symplectic integrators which preserves the symplectic structure. This last class is of particular interest when studying Hamiltonian and Lagrangian systems since the symplectic structure plays a crucial role in these systems[3,1,2]. The work done by Wisdom[36,37] on the $n$-body problem perfectly illustrates the benefits of such integrators.

At first, symplectic integrators were derived mostly as a subclass of Runge-Kutta algorithms for which the Runge-Kutta coefficients satisfy specific relationships [31]. Such a methodology, though very systematic, does not provide much physical insight and may be limited when we require several laws to be conserved. Other methods were developed in the 90’s, among which we may cite the use of generating functions for the canonical transformation induced by the phase flow[8,9] and the use of discrete variational principles. This last method “gives a comprehensive and unified view on much of the literature on both discrete mechanics as well as integration methods” (Marsden and West[26]). Names of variational principles differ in the literature, so we have decided to refer to Goldstein[10] in this paper: Hamilton’s principle concerns Lagrangian systems (i.e., refers to a principle of critical action that involves the Lagrangian) whereas the modified Hamilton’s principle concerns Hamiltonian systems (i.e., refers to a principle of critical action that involves the Hamiltonian). Several versions of the discrete modified Hamilton’s principle can be found in the literature such as the one developed by Shibberu[32] and Wu[38]. For the discrete Hamilton’s principle, Moser and Veselov[28] and then

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Marsden, West and Wendlandt [26, 35] developed a fruitful approach. Also, Jalnapurkar, Pekarsky and West [21] developed a variational principle on the cotangent bundle based on generating function theory.

In this paper, we focus on the discrete variational principles introduced by Guo, Li and Wu [15, 16, 17] because the theory they have developed provides both a discrete modified Hamilton’s principle (DMHP) and a discrete Hamilton’s principle (DHP) that are equivalent. We modify and generalize both variational principles they introduce by changing the time discretization so that a suitable analogue of the continuous boundary conditions may be enforced. These boundary conditions are crucial for the analysis of optimal control problems and play a fundamental role in dynamics. Our approach not only allows us to obtain a large class of discrete algorithms but it also gives new geometric insight into the Newmark model [29]. Most importantly, using our improved version of the discrete variational principles introduced by Guo et al., we develop a discrete Hamilton-Jacobi theory that yields new results on symplectic integrators.

In the first part of this paper (sections 2, 3 and 4), we present a discrete Hamilton’s principle on the tangent bundle and a discrete modified Hamilton’s principle on the cotangent bundle (section 2), we discuss the differences with other works on variational integrators (section 3) and show that we are able to recover classical symplectic schemes (section 4). The second part (sections 5 and 6) is devoted to issues related to energy conservation and energy error. We first show that by considering time as a generalized coordinate we can ensure energy conservation (section 5). Then we introduce the framework for discrete symplectic geometry and the notion of discrete canonical transformations. We obtain a discrete Hamilton-Jacobi theory that allows us to show that the energy error in the symplectic integration of a dynamical system is invariant under discrete canonical transformations (section 6). Finally, in the last part (section 7) we develop a discrete maximum principle that yields discrete necessary conditions for optimality. These conditions are in agreement with the usual conditions obtained from Pontryagin maximum principle and define symplectic algorithms that solve the optimal control problem.

In each part, we illustrate some of the ideas with simulations. In particular we show in the first part that symplectic methods allow one to recover the generating function from the phase flow while standard numerical integrators fail because they do not enforce the necessary exactness condition. The examples presented are the simple harmonic oscillator and a nonintegrable system describing a particle orbiting an oblate body. In the second part we look at the energy error in the integration of the equations of motion of a particle in a double well potential using a set of coordinates and its transform under discrete symplectic map. In the last part, we use the discrete maximum principle to study the Heisenberg optimal control problem.
2 Discrete principles of critical action: DMHP and DHP

In this section, we develop a modified version of both variational principles introduced by Guo, Li and Wu [15,16,17] and present the geometry associated with them.

2.1 Discrete geometry

Consider a discretization of the time $t$ into $n$ instants $\mathcal{T} = \{(t_k)_{k \in [1,n]}\}$. Here $t_{k+1} - t_k$ may not be equal to $t_k - t_{k-1}$ but for sake of simplicity we assume in the following that $t_{k+1} - t_k = \tau \ \forall k \in [1,n]$. The configuration space at $t_k$, is the $n$-dimensional manifold $M_k$ and $\mathcal{M} = \bigcup M_k$ is the configuration space on $\mathcal{T}$. Define a discrete time derivative operator $\Delta^d_{\tau}$ on $\mathcal{T}$. Note that $\Delta^d_{\tau}$ may not verify the usual Leibnitz law but a modified one. For instance, if we choose $\Delta^d_{\tau}$ to be the forward difference operator on $\mathcal{T}$:

$$\Delta^d_{\tau} q(t_k) := \frac{1}{\tau} (q(t_k + \tau) - q(t_k)) = \frac{q_{k+1} - q_k}{\tau} := \Delta^d \tau q_k$$

then $\Delta^d_{\tau}$ verifies:

$$\Delta^d_{\tau} (f(t)g(t)) = \Delta^d_{\tau} f(t) \cdot g(t) + f(t + \tau) \cdot \Delta^d_{\tau} g(t). \tag{1}$$

2.2 Discrete Hamilton’s principle

Our modified version of the discrete Hamilton’s principle derived by Guo, Li and Wu [15] is the discrete time counterpart of Hamilton’s principle for Lagrangian systems. Consider a discrete curve of points $(q^d_k)_{k \in [0,n]}$ and a discrete Lagrangian $L_d(q^d_k, \Delta^d_{\tau} q^d_k)$ where $\Delta^d_{\tau}$ is a discrete time derivative operator and $q^d_k$ is a function of $(q_k, q_{k+1})$.

**Definition 1 (Discrete Hamilton’s principle)** Trajectories of the discrete Lagrangian system $L_d$ going from $(t_0, q_0)$ to $(t_n, q_n)$ correspond to critical points of the discrete action

$$S^L_d = \sum_{k=0}^{n-1} L_d(q^d_k, \Delta^d_{\tau} q_k) \tau, \tag{2}$$

in the class of discrete curves $(q^d_k)_k$ whose ends are $(t_0, q_0)$ and $(t_n, q_n)$. In other words, if we require that the variations of the discrete action $S^L_d$ be zero for any choice of $\delta q^d_k$, and $\delta q_0 = \delta q_n = 0$, then we obtain discrete Euler-Lagrange equations.
Note that if we do not impose $t_{k+1} - t_k = t_k - t_{k-1}$, then the discrete action would be defined as:

$$S_d^L = \sum_{k=0}^{n-1} L_d(q^d_k, \Delta_r q_k)(t_{k+1} - t_k),$$

but the discrete Hamilton’s principle would be stated in the same manner\(^1\).

To proceed to the derivation of the equations of motion, we need to specify the derivative operator, $\Delta_r^d$. As we will explain below, its definition depends on the scheme we consider. We should also mention that our variational principle differs from Guo, Li and Wu’s since we consider that the action has only finitely many terms and we impose fixed end points. Such a formulation is more in agreement with continuous time variational principles and preserves the fundamental role played by boundary conditions. For a discussion on this topic, we refer to Lanczos [24] section 15.

### 2.3 Discrete modified Hamilton’s principle

As in the continuous case, there exists a discrete variational principle on the cotangent bundle that is equivalent to the above discrete Hamilton’s principle.

**Definition 2** Let $L_d$ be a discrete Lagrangian on $T\mathcal{M}$ and define the discrete Legendre transform (or discrete fiber derivative) $\mathbb{F}L : T\mathcal{M} \rightarrow T^*\mathcal{M}$ which maps the discrete state space $T\mathcal{M}$ to $T^*\mathcal{M}$ by

$$(q^d_k, \Delta_r q_k) \mapsto (q^d_k, p^d_k),$$

where

$$p^d_k = \frac{\partial L_d(q^d_k, \Delta_r q_k)}{\partial \Delta_r q_k}.$$  

If the discrete fiber derivative is a local isomorphism, $L_d$ is called regular and if it is a global isomorphism we say that $L_d$ is hyperregular.

If $L_d$ is hyperregular, we define the corresponding discrete Hamiltonian function on $T^*\mathcal{M}$ by

$$H_d(q^d_k, p^d_k) = \langle p^d_k, \Delta_r q_k \rangle - L_d(q^d_k, \Delta_r q_k),$$

\(^1\) In this formulation, the $t_k$’s are known, so there are no additional variables.
where $\Delta^d q^d_k$ is defined implicitly as a function of $(q^d_k, p^d_k)$ through equation (5). Let $S^H_d$ be the discrete action summation:

$$S^H_d = \sum_{k=0}^{n-1} \left( \langle p^d_k, \Delta^d \tau q^d_k \rangle - H_d(q^d_k, p^d_k) \right) \tau,$$

(7)

where $\tau$ is to be replaced by $t_{k+1} - t_k$ if $t_{k+1} - t_k \neq t_k - t_{k-1}$. Then the discrete principle of least action may be stated as follows:

**Definition 3 (Discrete modified Hamilton’s principle)** Trajectories of the discrete Hamiltonian system $H_d$ going from $(t_0, q_0)$ to $(t_n, q_n)$ correspond to critical points of the discrete action $S^H_d$ in the class of discrete curves $(q^d_k, p^d_k)$ whose ends are $(t_0, q_0)$ and $(t_n, q_n)$.

Again, for deriving the equations of motion we need to specify the discrete derivative operator, $\Delta^d_\tau$ and its associated Leibnitz law. It will generally depend upon the scheme we consider as we will see through examples later.

## 3 Comparison with other classical variational principle

At this point it is of interest to compare discrete variational principles introduced in this paper and other classical discrete variational principles. As we mentioned above, the discrete variational principles we develop are inspired by the work of Guo, Li and Wu [15] and we explained above the key difference between our work and this earlier work. We now point out the main differences of the work discussed here with that of Marsden and West, based on the variational principle introduced by Moser and Veselov. In the following, DVPI refers to the discrete variational principle developed by Moser, Veselov, Marsden, Wendlandt et al. whereas DVPII denotes the discrete variational principles developed by Guo and this paper.

The first main difference lies in the geometry of both variational principles. Whereas the discrete Lagrangian is a functional on $Q \times Q$ where $Q$ is the configuration space in DVPI, it is a functional on $TQ$ in DVPII. As a consequence, DVPII has a form more like that of the continuous case but has a major drawback: we have to specify the derivative operator and the Leibnitz law it verifies in order to derive discrete Euler-Lagrange equation. Such a law allows us to perform the discrete counterpart of the integration by parts and depends on the scheme we consider. On the other hand, the Euler-Lagrange equation obtained by DVPI is scheme independent. One benefit is that these equations ensure satisfaction of physical laws such as Noether’s theorem for any numerical scheme which can be derived from them.

The next important difference between the two discrete variational principles
lies in the role of the Legendre transformation in defining a discrete Hamiltonian function from the discrete Lagrangian. In DVPI, one defines a discrete Legendre transform to compute the momenta from the discrete Lagrangian function, so one may study the discrete dynamics on both $Q \times Q$ and $T^*Q$. However, it does not seem possible to define a discrete Hamiltonian function from the discrete Lagrangian and develop a DMHP. Given a Hamiltonian system, to derive discrete equations of motion using DVPI one needs to first find a continuous Lagrangian function by performing a Legendre transform on the continuous Hamiltonian function, then apply DVPI and finally use the discrete Legendre transform to study the dynamics on $T^*Q$ (see for instance [26] page 408). While this point may not be of importance when dealing with dynamical systems, it is crucial if one wants to discretize an optimal control problem, where the continuous Hamiltonian function does not have any physical meaning and the Legendre transformation may not be well-defined (See section 7). DVPII naturally defines a discrete Legendre transform and a DMHP.

As mentioned in the introduction, people have already introduced DMHPs on the cotangent bundle, but, as far as we know, no one has developed an approach that allows one to equivalently consider both the Hamiltonian and Lagrangian approaches in discrete settings (i.e., a DMHP and a DHP that are equivalent for non-degenerate Lagrangian systems). In addition, the DMHPs that can be found in the literature do not allow one to recover most of the classical schemes. For instance, Shibberu’s DMHP focuses on the midpoint scheme and Wu developed a different DMHP for each scheme.

Let us now look at some classical schemes and see how they can be derived from DVPII.

4 Examples

4.1 Störmer’s rule and Newmark methods

Störmer’s scheme is a symplectic algorithm that was first derived for molecular dynamics problems. It can be viewed as a Runge-Kutta-Nyström method induced by the leap-frog partitioned Runge-Kutta method[31]. The derivation of Störmer rule as a variational integrator came later and can be found in [38,35]. Guo, Li and Wu [17] recovered this algorithm using their discrete variational principles. In the next subsection, we briefly go through the derivation and add to their work the velocity Verlet [34] and Newmark methods[26]. In particular, we will show how the conservation of the Lagrangian and symplectic two-form is built into DVPII.
4.1.1 From the Lagrangian point of view

We first let $q^d_k = q_k$ and define the discrete Lagrangian by $L_d(q_k^d, \Delta^d_q k) = L(q_k, \Delta^d_q k)$ and the discrete derivative operator as the forward difference $\Delta^d q = \Delta q$. $\Delta q$ satisfies the modified Leibnitz law (1). Discrete equations of motion are obtained from discrete Hamilton’s principle (definition (1)):

$$\delta S^L_d = \tau \sum_{k=0}^{n-1} \delta L_d(q_k, \Delta q_k)$$

$$\delta S^L_d = \tau \sum_{k=0}^{n-1} \langle D_1 L_d(q_k, \Delta q_k), \delta q_k \rangle + \langle D_2 L_d(q_k, \Delta q_k), \delta \Delta q_k \rangle$$

$$\delta S^L_d = \tau \sum_{k=1}^{n-1} \langle D_1 L_d(q_k, \Delta q_k) - \Delta q D_2 L_d(q_{k-1}, \Delta q_{k-1}), \delta q_k \rangle$$

$$\delta S^L_d = \tau \sum_{k=1}^{n-1} \langle D_1 L_d(q_k, \Delta q_k) - \Delta q D_2 L_d(q_{k-1}, \Delta q_{k-1}), \delta q_k \rangle$$

$$\delta S^L_d = \tau \sum_{k=1}^{n-1} \langle D_1 L_d(q_k, \Delta q_k) - \Delta q D_2 L_d(q_{k-1}, \Delta q_{k-1}), \delta q_k \rangle$$

$$\delta S^L_d = \tau \sum_{k=1}^{n-1} \langle D_1 L_d(q_k, \Delta q_k) - \Delta q D_2 L_d(q_{k-1}, \Delta q_{k-1}), \delta q_k \rangle$$

where the commutativity of $\delta$ and $\Delta q$ and the modified Leibnitz law defined by equation (1) have been used.

Discrete Euler-Lagrange equations follow by requiring the variations of the action to be zero for any choice of $\delta q_k$, $k \in [1, n - 1]$ and $\delta q_0 = \delta q_n = 0$:

$$D_1 L_d(q_k, \Delta q_k) - \Delta q D_2 L_d(q_{k-1}, \Delta q_{k-1}) = 0.$$  (12)

Suppose $L(q, \dot{q}) = \frac{1}{2} q M \dot{q} - V(q)$, then equation (12) yields Störmer’s rule:

$$q_{k+1} = 2q_k - q_{k-1} + h^2 M^{-1}(-\nabla V(q_k)).$$  (13)

Consider the one-form

$$\theta^L_i = \frac{\partial L_d(q_{k-1}, \Delta q_{k-1})}{\partial \Delta q_{k-1}} dq_i,$$

and define the Lagrangian two-form $\omega^L_i$ on $T_{q_k} \mathcal{M}$:

---

2 Einstein’s summation convention is assumed
\[ \omega^L_k = d\theta^L_k = \frac{\partial^2 L_d(q_{k-1}, \Delta_rq_{k-1})}{\partial q^i_{k-1} \partial \Delta_r q^i_{k-1}} dq^i_k \wedge dq^j_k + \frac{\partial^2 L_d(q_{k-1}, \Delta_rq_{k-1})}{\partial \Delta_r q^i_{k-1} \partial \Delta_r q^j_{k-1}} dq^i_k \wedge dq^j_k. \] (14)

**Lemma 4** The algorithm defined by Störmer’s rule preserves the Lagrangian two-form, \( \omega^L_k \).

**PROOF.** Consider a discrete trajectory \((q_k)_k\) that verifies equation (13). Then we have:

\[
dS^L_d = \tau \sum_{k=1}^{n-1} \left( \frac{\partial L_d(q_k, \Delta_rq_k)}{\partial q^i_k} - \Delta_r \frac{\partial L_d(q_{k-1}, \Delta_rq_{k-1})}{\partial \Delta_r q^i_{k-1}} \right) dq^i_k \\
+ \Delta_r \left( \frac{\partial L_d(q_{k-1}, \Delta_rq_{k-1})}{\partial \Delta_r q^i_{k}} dq^i_k \right). \tag{15}
\]

Since the \(q_k\)'s verify equation (13), and \(d^2 = 0\), equation (15) yields:

\[ d(\Delta_r \theta^L_k) = 0, \] that is, \( \omega^L_{k+1} = \omega^L_k \). (16)

We conclude that \( \omega^L_k \) is preserved along the discrete trajectory.

As we mentioned earlier, because DVPII acts on the tangent bundle it provides results very similar to the continuous case as attested by the form of the Lagrangian 2-form. This is to be compared with the Lagrangian two-form arising in the continuous case:

\[ \omega^L = \frac{\partial^2 L}{\partial q^i \partial \dot{q}^j} dq^i \wedge dq^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} d\dot{q}^i \wedge d\dot{q}^j. \] (17)

Note that conservation of the Lagrangian two-form is a consequence of using the Leibnitz law, and therefore does not depend on the definition of the discrete Lagrangian. In the remainder of this section we use different discrete Lagrangian functions, but the same Leibnitz law. Thus lemma 4 still applies.

More generally, we can derive Störmer’s rule using

\[ L_d(q_k, \Delta_rq_k) = \lambda L(q_k, \Delta_rq_k) + (1 - \lambda)L(q_k + \tau \Delta_rq_k, \Delta_rq_k), \]

for any \( \lambda \) in \( \mathbb{R} \). A particular case of interest is \( \lambda = \frac{1}{2} \) which yields a symmetric version of Störmer’s rule also called the velocity Verlet method[34]. For this value of \( \lambda \), we define the associated discrete momenta using the Legendre transform (equation (5)): 
\[ p_{k+1} = p_k^d \]
\[ = D_2 L_d(q_k, \Delta_r q_k) \]  
\[ = M \Delta_r q_k - \frac{1}{2} \tau \nabla V(q_k + \Delta_r q_k), \]  
that is:
\[ q_{k+1} = q_k + \tau M^{-1}(p_{k+1} + \frac{1}{2} \tau \nabla V(q_{k+1})). \]  
Moreover, from equation (12) we obtain:
\[ p_{k+1} = p_k + \tau \frac{-\nabla V(q_k) - \nabla V(q_{k+1})}{2}. \]
Equations (21) and (22) define the velocity Verlet algorithm.

We now focus on the Newmark algorithm which is usually written for the system \( L = \frac{1}{2} q^T M \ddot{q} - V(q) \) as a map given by \((q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1})\) satisfying the implicit relations:
\[ q_{k+1} = q_k + \tau \dot{q}_k + \frac{\tau^2}{2} [(1 - 2\beta) a_k + 2\beta a_{k+1}], \]  
\[ \dot{q}_{k+1} = \dot{q}_k + \tau [(1 - \gamma) a_k + \gamma a_{k+1}], \]  
\[ a_k = M^{-1}(-\nabla V(q_k)), \]
where the parameters \( \gamma \in [0, 1] \) and \( \beta \in [0, \frac{1}{2}] \). For \( \gamma = \frac{1}{2} \) and any \( \beta \) the Newmark algorithm can be generated from DVPII as a particular case of the Störmer rule where \( q_k^d \) and \( L_d \) are chosen as follows:
\[ q_k^d = q_k - \beta \tau^2 a_k, \]
and
\[ L_d(q_k^d, \Delta_r q_k^d) = \frac{1}{2} q_k^d T M q_k^d - \tilde{V}(q_k^d), \]
with \( \tilde{V} \), the modified potential, satisfying \( \nabla \tilde{V}(q_k^d) = \nabla V(q_k) \). Since the derivative operator is the same as above, the discrete Hamilton’s principle yields Störmer’s equation where \( q_k \) is replaced by \( q_k^d \), that is:
\[ q_{k+1}^d = 2q_k^d - q_{k-1}^d + \tau^2 M^{-1}(-\nabla \tilde{V}(q_k^d)). \]  
Equation (26) simplifies to
\[ q_{k+1} - 2q_k + q_{k-1} = \tau^2 (\beta a_{k+2} + (1 - 2\beta) a_{k+1} + \beta a_{k-1}). \]  
This last equation corresponds to the Newmark algorithm for the case \( \gamma = \frac{1}{2} \). Lemma 4 guarantees that the Lagrangian two-form
\[ \omega_k^L = d(D_2 L_d(q_k^d, \Delta_r q_k^d) dq_{k+1}^d) \]
is preserved along the discrete trajectory.
4.1.2 From the Hamiltonian point of view

The Störmer, velocity Verlet, and Newmark algorithms can also be derived using a phase space approach, i.e., the DMHP. For Störmer’s rule, the Legendre transform yields:

\[ p_{k+1} = M \Delta \tau q_k . \]

(28)

The discrete Hamiltonian function is defined from equation (6):

\[ H_d(q_k, p_{k+1}) = \frac{1}{2} p_{k+1}^T M^{-1} p_{k+1} + V(q_k) , \]

(29)

and discrete equations of motion are obtained from the DMHP\(^3\) (theorem (3)). We skip a few steps in the evaluation of the variations of \( S^H_d \) to finally find:

\[
\delta S^H_d = \delta \left( \tau \sum_{k=0}^{n-1} \langle p_{k+1}, \Delta \tau q_k \rangle - H_d(q_k, p_{k+1}) \right) \\
= \tau \sum_{k=0}^{n-1} \langle \Delta \tau q_k - D_2 H_d(q_k, p_{k+1}), \delta p_{k+1} \rangle - \langle \Delta \tau p_k + D_1 H_d(q_k, p_{k+1}), \delta q_k \rangle \\
+ \langle p_n, \delta q_n \rangle - \langle p_0, \delta q_0 \rangle .
\]

(30)

(31)

If we impose the variations of the action \( S^H_d \) to be zero for any \((\delta q_k, \delta p_{k+1})\) and \(\delta q_0 = \delta q_n = 0\), we obtain:

\[
\Delta \tau q_k = p_{k+1} , \\
\Delta \tau p_k = -\nabla V(q_k) .
\]

(32)

(33)

Elimination of the \( p_k \)’s yields Störmer’s rule.

To recover the velocity Verlet scheme from the Hamiltonian point of view, one needs to solve for \( \Delta \tau q_k \) as a function of \((q_k, p_{k+1})\) in equation (20). Suppose this has been done and that \( \Delta \tau q_k = f(q_k, p_{k+1}) \), then

\[
H_d(q_k, p_{k+1}) = \langle p_{k+1}, f(q_k, p_{k+1}) \rangle - L_d(q_k, f(q_k, p_{k+1})) .
\]

(34)

Taking the variation of the action \( S^H_d \) yields the following discrete Hamilton’s equations:

\[
\Delta \tau q_k = D_2 H_d(q_k, p_{k+1}) , \\
\Delta \tau p_k = -D_1 H_d(q_k, p_{k+1}) .
\]

(35)

(36)

\(^3\) \( q^d_k = q_k \) and \( p^d_k = p_{k+1} \)
On the other hand, equation (34) provides the following relationships:

\[
D_1 H_d(q_k, p_{k+1}) = D_1 f(q_k, p_{k+1})(p_{k+1} - D_2 L_d(q_k, f(q_k, p_{k+1})))
- D_1 L_d(q_k, f(q_k, p_{k+1})), \quad (37)
\]

\[
D_2 H_d(q_k, p_{k+1}) = \Delta^d_r q_k + D_2 f(q_k, p_{k+1})(p_{k+1} - D_2 L_d(q_k, f(q_k, p_{k+1}))). \quad (38)
\]

Combining equations (35) and (36) together with equations (37) and (38) yields the Velocity Verlet algorithm (equations (21) and (22)).

We now prove that the scheme we obtained is symplectic. As in the Lagrangian case, the proof differs from the usual one that consists in computing \( dp_{k+1} \wedge dq_k \), in that it relies on fundamental properties of DVPII and on the use of the Leibnitz law.

**Lemma 5** The algorithm defined by equations (35)-(36) is symplectic.

**PROOF.** We have:

\[
dS^H_d = d \left( \tau \sum_{k=0}^{n-1} \langle p_{k+1}, \Delta^r q_k \rangle - H_d(q_k, p_{k+1}) \right), \quad (39)
\]

\[
= \tau \sum_{k=0}^{n-1} \langle \Delta^r q_k - D_2 H_d(q_k, p_{k+1}), dp_{k+1} \rangle - \langle \Delta^r p_k + D_1 H_d(q_k, p_{k+1}), dq_k \rangle
+ \Delta^r \langle p_k, dq_k \rangle. \quad (40)
\]

Hence, since \((q_k, p_k)\) verifies equations (35)-(36) and \(d^2 = 0\), we obtain:

\[
\Delta^r (dp_k \wedge dq_k) = 0. \quad (41)
\]

The symplectic two-form \(dp_k \wedge dq_k\) is preserved along the trajectory.

Finally, we can also derive the Newmark methods from the Hamiltonian point of view. The Legendre transform yields:

\[
p^d_k = \frac{\partial L_d(q^d_k, \Delta^d_r q^d_k)}{\partial \Delta^d_r q^d_k} = M \Delta^d_r q^d_k. \quad (42)
\]

The Newmark algorithm is again a particular case of the Störmer rule where \((q_k, p_{k+1})\) is replaced by \((q^d_k, p^d_k)\):

\[
\Delta^d_r q^d_k = p^d_k, \quad (43)
\]

\[
\Delta^d_r p^d_k = -\nabla \tilde{V}(q^d_k). \quad (44)
\]
Defining \( \dot{q}_k \) from \( p_k \) as
\[
\dot{q}_k = M^{-1}p_k^d + \frac{\tau}{2} a_k
\]
allows us to recover the Newmark scheme for \( \gamma = \frac{1}{2} \) (equations (23) and (24)). From the above lemma, we obtain that the symplectic two-form \( dp_k^d \wedge dq_k^d \) is preserved along the trajectory.

4.2 Midpoint rule

The midpoint rule has been extensively studied and a complete study of its properties can be found in the literature. It is a particular case of the Runge-Kutta algorithm, but can also be derived as a variational integrator (see for instance [38,32,26]). The derivation of this scheme has been done by Guo, Li and Wu [17] for the Hamiltonian point of view. In the next section we present the Lagrangian point of view and then recall the Guo, Li and Wu main results, the goal of this section being to illustrate the use of DVPII with other discretization and discrete derivative operator.

4.2.1 From the Lagrangian point of view

Given a Lagrangian \( L(q, \dot{q}) \), define the discrete Lagrangian by:
\[
L_d(q_k^d, \Delta q_k^d) = L(q_k^d, \Delta_q q_k),
\]
where \( q_k^d = \frac{q_{k+1}^d + q_k^d}{2} \), and \( \Delta_q = R_{\tau/2} - R_{-\tau/2} \) where the operator \( R_\tau \) is the translation by \( \tau \). One can readily verify that \( \Delta_q q_k^d = \Delta_q q_k \) and that \( \Delta_q^d \) verifies the usual Leibnitz law:
\[
\Delta_q^d(f_k^d g_k^d) = \Delta_q f_k^d \cdot g_k^d + f_k^d \cdot \Delta_q g_k^d,
\]
where \( f_k = f(t_k) \) and \( g_k = g(t_k) \) are functions of time and \( f_k^d = \frac{f_{k+1}^d + f_k^d}{2} \).

Applying the discrete Hamilton's principle yields:
\[
\delta S^L_d = \tau \sum_{k=0}^{n-1} \delta L_d(q_k^d, \Delta q_k^d) = \tau \sum_{k=0}^{n-1} \langle D_1 L_d(q_k^d, \Delta q_k^d), \delta q_k^d \rangle + \langle D_2 L_d(q_k^d, \Delta q_k^d), \delta \Delta q_k^d \rangle.
\]

From the Legendre transform (equation (5)), we define the associated momentum:
\[
\frac{p_{k+1}^d + p_k^d}{2} = p_k^d = D_2 L_d(q_k^d, \Delta q_k^d).
\]
Then, equation (48) becomes:

$$
\delta S^L_d = \tau \sum_{k=0}^{n-1} \langle D_1 L_d(q^d_k, \Delta^d_q q^d_k), \delta q^d_k \rangle + \langle p^d_k, \delta \Delta^d_q q^d_k \rangle 
= \tau \sum_{k=0}^{n-1} \langle D_1 L_d(q^d_k, \Delta^d_q q^d_k) - \Delta^d_q p^d_k, \delta q^d_k \rangle + \langle p_n, \delta q_n \rangle - \langle p_0, \delta q_0 \rangle. 
$$

If we require the variations of the action to be zero for any choice of $\delta q^d_k$, $k \in [1, n-1]$, and $\delta q_0 = \delta q_n = 0$, we obtain discrete Euler-Lagrange equations for the midpoint scheme:

$$
p_{k+1} - p_k \frac{h}{h} = \Delta^d_q p^d_k 
= D_1 L_d(q^d_k, \Delta^d_q q^d_k) 
= D_1 L_d\left(\frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{h}\right), 
$$

$$
p_{k+1} + p_k \frac{2}{2} = p^d_k 
= D_2 L_d(q^d_k, \Delta^d_q q^d_k) 
= D_2 L_d\left(\frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{h}\right). 
$$

**Lemma 6** The midpoint scheme defines a symplectic algorithm.

**PROOF.** The proof proceeds as for the Störmer rule:

$$
dS^L_d = \tau \sum_{k=0}^{n-1} \langle D_1 L_d(q^d_k, \Delta^d_q q^d_k), dq^d_k \rangle + \langle p^d_k, d\Delta^d_q q^d_k \rangle 
= \tau \sum_{k=0}^{n-1} \langle D_1 L_d(q^d_k, \Delta^d_q q^d_k) - \Delta^d_q p^d_k, dq^d_k \rangle + \Delta^d_q \langle p^d_k, dq^d_k \rangle. 
$$

Since $d^2 = 0$ and $(q_k, p_k)$ verifies equations (52)-(53), we obtain:

$$
\Delta^d_q (dp^d_k \wedge dq^d_k) = 0. 
$$

A straightforward computation shows that $\Delta^d_q (dp^d_k \wedge dq^d_k) = \Delta^d_q (dp_k \wedge dq_k)$, i.e., the symplectic two-form $\omega_k = dp_k \wedge dq_k$ is preserved along the trajectory.

**4.2.2 From the Hamiltonian point of view**

Let $H_d(q^d_k, p^d_k) = H(q^d_k, p^d_k)$ or equivalently define $H_d$ from $L_d$ via equation (6) and let $(q_k^d, p_k^d) = (\frac{q_k + q_{k+1}}{2}, \frac{p_k + p_{k+1}}{2})$. Then the DMHP (3) yields:
\[ \frac{q_{k+1} - q_k}{\hbar} = \Delta_r \frac{p^d}{p_k} = D_2 H_d(q^d_k, p^d_k) = \frac{\partial H}{\partial p} \left( \frac{q_{k+1} + q_k}{2}, \frac{p_{k+1} + p_k}{2} \right), \]  
(57)

\[ \frac{p_{k+1} - p_k}{\hbar} = \Delta_r \frac{p^d}{p_k} = -D_1 H_d(q^d_k, p^d_k) = -\frac{\partial H}{\partial q} \left( \frac{q_{k+1} + q_k}{2}, \frac{p_{k+1} + p_k}{2} \right). \]  
(58)

**Lemma 7** The midpoint scheme defines a symplectic algorithm.

**PROOF.** The proof is straightforward. We compute \( d^2 S^H_d \) assuming \((q_k, p_k)\) verifies the above equations of motion.

To conclude, we have illustrated the use of the discrete variational principles (definitions (1) and (3)) and derived discrete equations of motion. One can readily verify that both variational principles yield the same discrete equations, as in the continuous case. Other schemes can be recovered in the same way, and we do not know yet if all classical symplectic algorithms can be derived from DVPII. For instance, we have been able to recover the conditions for the partitioned Runge-Kutta algorithm to be symplectic from the Lagrangian point of view but so far it is not clear to us how it can be done using the Hamiltonian approach (definition (3)).

### 4.3 Numerical example

Symplectic integrators are usually used as numerical integrators that preserve the qualitative behavior of dynamical systems and are especially valuable for long time simulations. However, these are not the only uses of symplectic integrators. In this section we present an aspect of symplectic integrators that we have not seen pointed out in the literature: we show that they allow one to recover the generating functions for the phase flow canonical transformation, whereas numerical integrators do not, even over a short period of time (applications of this result can be found in [14]).

Let us first recall two results from the Hamilton-Jacobi theory.

**Proposition 8** The transformation induced by the phase flow is canonical.
Proposition 9 Let \((P_1, \omega_1)\) and \((P_2, \omega_2)\) be symplectic manifolds, \(\pi_i : P_1 \times P_2 \to P_i\) the projection onto \(P_i\), \(i = 1, 2\), and

\[
\Omega = \pi_1^*\omega_1 - \pi_2^*\omega_2. \tag{59}
\]

Then:

(1) \(\Omega\) is a symplectic form on \(P_1 \times P_2\);

(2) a map \(f : P_1 \to P_2\) is symplectic if and only if \(i_f^*\Omega = 0\), where \(i_f : \Gamma_f \to P_1 \times P_2\) is inclusion and \(\Gamma_f\) is the graph of \(f\).

Hence, by the Poincaré lemma, if \(f\) is canonical there exists a function \(S\) such that

\[
i_f^*\Theta = dS, \tag{60}
\]

where \(\Omega = -d\Theta\). \(S\) is called a generating function. If \((q_i, p_i)\) are coordinates on \(P_1\) and \((Q^i, P_i)\) are coordinates on \(P_2\), then \(\Gamma_f\) can be endowed with a chart in several ways. For instance, \(S\) may appear as a function of \((q_i, Q^i)\) or of \((q_i, P_i)\), and so forth depending of the choice of \(\Theta\). Let \(\theta_1 = p_i dq^i\) and \(\theta_2 = P_i dQ^i\), then

\[
i_f^*\Theta = i_f^*\pi_1^*\theta_1 - i_f^*\pi_2^*\theta_2 = (\pi_1 \circ i_f)^* p_idq^i - (\pi_2 \circ i_f)^* P_idQ^i. \tag{61}
\]

In this case, \(S\) is a function of \((q^1, \ldots, q^n, Q^1, \ldots, Q^n)\). From

\[
dS = \frac{\partial S}{\partial q^i} dq^i + \frac{\partial S}{\partial Q^i} dQ^i,
\]

we conclude, using equation (60) that:

\[
p_i = \frac{\partial S}{\partial q_i}, \quad P_i = -\frac{\partial S}{\partial Q^i}, \tag{61}
\]

Suppose that \(f\) is the phase flow \(\Phi\), then equation (61) defines a relationship between flow and the gradient of the generating function. In particular, if the generating function \(S(q, q_0, t)\) exists and the flow is defined as follows:

\[
\Phi : (q_0, p_0, t) \mapsto (q(t), p(t)) = (\Phi_1(q_0, p_0), \Phi_2(q_0, p_0)), \tag{62}
\]

then, from the local inverse function theorem\(^4\), there exist two functions \(S_1\) and \(S_2\) such that:

\[
p_0 = S_1(q, q_0, t), \tag{63}
\]

\[
p = \Phi_2(q_0, S_1(q, q_0, t)) \equiv S_2(q, q_0, t). \tag{64}
\]

From equation (61), we conclude that \(S_1\) and \(S_2\) are the gradient of \(S\) and

\[\frac{\partial \Phi}{\partial p_0} \neq 0\] since we assume that \(S\) exists.
therefore should verify\(^5\):
\[
\frac{\partial^2 S}{\partial q_0 \partial q} \equiv \frac{\partial S_1}{\partial q} (q, q_0, t) = \frac{\partial S_2}{\partial q_0} (q, q_0, t) \equiv \frac{\partial^2 S}{\partial q \partial q_0}.
\] (65)

Since symplectic integrators preserve the symplectic two-form, the exactness condition (equation (65)) is satisfied whereas it is not using numerical integrators.

### 4.3.1 Harmonic Oscillator

We start with a trivial example, the harmonic oscillator, because its study allows us to introduce techniques and discuss issues that arise in the next more sophisticated example. The Hamiltonian function for the harmonic oscillator is quadratic:
\[
H(q, p) = \frac{1}{2m} p^2 + \frac{k}{2} q^2.
\] (66)

It is a linear system so the phase flow is also linear:
\[
\begin{align*}
\Phi_1(q_0, p_0) &= a_{11}(t)q_0 + a_{12}(t)p_0 \\
\Phi_2(q_0, p_0) &= a_{21}(t)q_0 + a_{22}(t)p_0.
\end{align*}
\] (67) (68)

Substituting these expressions into Hamilton’s equations and balancing terms of the same order yield:
\[
\begin{align*}
\dot{a}_{11}(t) &= \frac{a_{21}(t)}{m} \\
\dot{a}_{12}(t) &= \frac{a_{22}(t)}{m} \\
\dot{a}_{21}(t) &= ka_{11}(t) \\
\dot{a}_{22}(t) &= ka_{12}(t)
\end{align*}
\] (69)

In figure 1, we plot \(\Delta = \frac{\partial S_1}{\partial q} (q, q_0, t) - \frac{\partial S_2}{\partial q_0} (q, q_0, t)\) over the time interval \([0, 100]\) using the midpoint scheme with fixed time step, a symplectic Gauss implicit Runge-Kutta algorithm of order 8 with fixed time step and a non symplectic Runge-Kutta integrator of order 8 to integrate equations (69). We remark that only symplectic integrators allow us to recover the generating functions because the exactness condition is exactly verified. We point out that even over a short time span, numerical integrators fail to satisfy the exactness condition.

\(^5\) Since their exists an open set on which the generating functions are smooth, Schwartz’s theorem yields \(\frac{\partial^2 S}{\partial q_0 \partial q} = \frac{\partial^2 S}{\partial q \partial q_0}\).
(a) Midpoint scheme with fixed time step $\tau = 0.01$

(b) Implicit Gauss Runge-Kutta algorithm of order 8

(c) Explicit Runge-Kutta algorithm of order 8

Fig. 1. Exactness condition using 3 different integrators

4.3.2 Earth orbit

This example was first encountered by V.M. Guibout and D.J. Scheeres [12,14] while studying spacecraft formation flight. Consider an orbital problem about the Earth modelled by a non-spherical body (we take into account $J_2$ and $J_3$ gravity coefficients). The Hamiltonian of the system is given by

$$H = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) - \frac{1}{\sqrt{x^2 + y^2 + z^2}} \left(1 - \frac{R^2}{2r_0^2(x^2 + y^2 + z^2)} \left(3 \frac{z^2}{x^2 + y^2 + z^2} - 1\right) J_2 - \frac{R^3}{2r_0^3(x^2 + y^2 + z^2)^2} \left(5 \frac{z^3}{x^2 + y^2 + z^2} - 3z\right) J_3 \right) , \quad (70)$$

where

$$GM = 398,600.4405 \ km^3 s^{-2}, \quad R = 6,378.137 \ km ,$$

$$J_2 = 1.082626675 \cdot 10^{-3} , \quad J_3 = 2.532436 \cdot 10^{-6} ,$$
and all the variables are normalized ($r_0$ is the initial radius of a trajectory):

\[
x \rightarrow x r_0, \quad y \rightarrow y r_0, \quad z \rightarrow z r_0, \quad t \rightarrow t \sqrt{\frac{r_0^3}{GM}}, \quad p_x \rightarrow p_x \sqrt{\frac{GM}{r_0}}, \quad p_y \rightarrow p_y \sqrt{\frac{GM}{r_0}}, \quad p_z \rightarrow p_z \sqrt{\frac{GM}{r_0}}.
\]  

(71)

We choose the nominal trajectory to be a highly eccentric orbit. The initial conditions for the nominal trajectory are in normalized units ($r_0 = 7000$ km):

\[
x = 1, \quad y = 0, \quad z = 0, \quad p_x = 0, \quad p_y = \sqrt{\frac{13}{10}} \cos(\pi/3), \quad p_z = v \sqrt{\frac{13}{10}} \sin(\pi/3).
\]  

(72)

At the initial time, $e = 0.3, i = \frac{\pi}{3}$ rad, $\omega = 0$ and $\Omega = 0$.

This system is non-integrable and has non-trivial dynamics. The phase flow is not known globally but techniques have been developed to evaluate it locally (see Guibout and Scheeres [13]).

Consider a given trajectory called the nominal trajectory ($q^0(t), p^0(t)$), then the dynamics of the relative motion of a particle about this trajectory is Hamiltonian and is described by the following Hamiltonian function $H^h(X^h, t)$:

\[
\sum_{p=2}^{\infty} \sum_{i_1, \ldots, i_{2n}=0}^{p} \frac{1}{i_1! \cdots i_{2n}!} \frac{\partial^p H}{\partial q_1^{i_1} \cdots \partial q_n^{i_n} \partial p_1^{i_{n+1}} \cdots \partial p_2^{i_{2n}}}(q^0, p^0, t)X_1^{i_1} \cdots X_{2n}^{i_{2n}},
\]  

(73)

where $X^h$ is the relative state vector ($\Delta q, \Delta p$).

In the same way, we expand in Taylor series the phase flow for the relative motion, and substitute its expression into Hamilton’s equations for $H^h$. When studying spacecraft formation flight we often assume that the spacecraft stay close to each other and therefore, one may approximate the dynamics of the formation by truncating the above Taylor series. Suppose we keep only terms of order less that $N$. Then balancing terms of the same order in Hamilton’s equations yields a set of ordinary differential equations (the procedure is the same as in the harmonic oscillator example but here there are non-linear terms up to order $N$). We use the midpoint scheme with fixed-time step ($\tau = 0.01$), a symplectic Gauss implicit Runge-Kutta algorithm of order 4 with fixed time step ($\tau = 0.01$) and Mathematica© built-in numerical integrator NDSolve to integrate the flow up to order $N = 4$. Once the Taylor series of the flow is known, we find $S_1$ and $S_2$ by a series inversion. Then we check the exactness conditions defined by equation (65) (there are several terms involved since we are dealing with a nonlinear system of dimension 6). We find that after

6 NDSolve switches between a non-stiff Adams method and a stiff Gear method.
10\pi units of time, $\|\frac{\partial S}{\partial q} - \frac{\partial S}{\partial q_0}\| \leq \eta$, where $\eta = 10^{-11}$ using the midpoint scheme, $\eta = 10^{-11}$ with the symplectic implicit Gauss Runge-Kutta algorithm and $\eta = 10^{-3}$ with the built-in function NDSolve. Again, only symplectic algorithms allow us to recover the generating functions.

5 Energy conservation

Symplectic integrators do not conserve energy and in general induce bounded energy error. There are several works on analyzing the energy error, we refer to Hairer and Lubich [19] and Hairer, Lubich and Wanner [20] and references therein for more details. In this section, we enhance DVPII so that energy conservation is imposed. By considering the time as a coordinate and by adding an independent parameter $\tau$, DVPII yields symplectic energy conserving algorithms. For certain problems, such algorithms may provide better performance\(^7\), but the contrary may also happen [18,33]. The method we develop in this section is variational and allows us to recover Shibberu’s algorithm [32] for Hamiltonian systems and is equivalent to the Kane, Marsden and Ortiz [23] method for Lagrangian systems.

5.1 Generalized variational principles

5.1.1 Generalized Hamilton’s principle

Let us first recall Hamilton’s principle for dynamical systems for which time is considered as a generalized coordinate. Such a formulation is typically used in relativity where the time coordinate is equivalent to the space coordinates.

Consider a Lagrangian $L(q, \dot{q})$ and define the **parametric** Lagrangian

\[
\bar{L}(q, t, q', t') = t' L(q, \frac{q'}{t'}, t),
\]

where $' = \frac{d}{d\tau}$ and $\tau$ is an independent parameter that parameterizes the trajectory and the time. Then the generalized Hamilton’s principle reads:

**Definition 10** Critical points of $\int_{t_0}^{t_f} \bar{L}(q, \frac{q'}{t'}, t) d\tau$ in the class of curves $(q(\tau), t(\tau))$ with endpoints $(q_0, t_0)$ and $(q_f, t_f)$ correspond to trajectories of the Lagrangian systems going from $(q_0, t_0)$ to $(q_f, t_f)$.

\(^7\) To quantify the performance of an algorithm, not only we look at its accuracy but we also evaluate its ability to predict the qualitative behavior of the system. In that sense, symplectic-energy conserving algorithms may not predict qualitative behavior better that symplectic algorithms.
The generalized Hamilton’s principle yields the following set of equations:

\[
\frac{\partial \bar{L}}{\partial t} - \frac{d}{d\tau} \frac{\partial \bar{L}}{\partial t'} = 0, \quad (74)
\]

\[
\frac{\partial \bar{L}}{\partial q} - \frac{d}{d\tau} \frac{\partial \bar{L}}{\partial \dot{q}} = 0. \quad (75)
\]

Replacing the parametric Lagrangian by the Lagrangian of the system simplifies the above equations to:

\[
t' \frac{\partial L}{\partial t} - \frac{d}{d\tau} L + \frac{d}{d\tau} \left( \frac{\partial L q'}{\partial \dot{q}} \right) = 0, \quad (76)
\]

\[
t' \frac{\partial L}{\partial q} - \frac{d}{d\tau} \frac{\partial L}{\partial \dot{q}} = 0. \quad (77)
\]

These \(n + 1\) equations should be compared to the \(n\) equations obtained when the trajectory is parameterized by the time:

\[
\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0. \quad (78)
\]

Since \(\frac{d}{d\tau} = t' \frac{d}{dt}\), we conclude that the space components of the generalized Euler-Lagrange equations (equation (77)) are a multiple by \(t'\) of the original Euler-Lagrange equations (equation (78)). Also, their time component (equation (76)) is a linear combination of the components of equation (78) (the sum of each component multiplied by \(q'\)). All \(n + 1\) generalized Euler-Lagrange equations are thus consistent with the original equations but there is no unique solution because they are satisfied by any parameterization. To get a unique solution, it is necessary to add to the generalized Hamilton’s principle an additional condition fixing the parameterization. As we will see in the next section, in discrete settings we do not have this freedom anymore. The discrete counter-part of equation (76) corresponds to an energy constraint that fully specifies the time parameterization, i.e., the time step.

5.1.2 Generalized discrete Hamilton’s principle (GDHM)

In contrast with the variational principles introduced in the first part of this paper, we do not set the time step, i.e., we let the time act as a variable by adding an independent parameter \(\tau_k\) such that \(t_k = t(\tau_k)\) and \(\tau_{k+1} - \tau_k = \tau\), \(\tau\) being a constant. \(t_k\) is now a coordinate that plays the same role as \(q_k\), \(M_k\) is the extended configuration space \((q_k, t_k)\), \(M = \bigcup M_k\) and \(\mathcal{T} = \{(\tau_k)_{k\in[1,n]}\}\.21
Define the modified discrete Lagrangian $\bar{L}_d$:

$$\bar{L}_d(q^d_k, t^d_k, \Delta_q^d q^d_k, \Delta_t^d t^d_k) = \Delta_t^d t^d_k \frac{\Delta_q^d q^d_k}{\Delta_t^d t^d_k},$$  \quad (79)$$

where $L_d$ is the discrete Lagrangian previously defined. In addition, since we are interested in conservation of energy we only consider system that are time independent. As a consequence, $L_d$ does not depend on time and $\frac{\partial L_d}{\partial q_k} = 0$.

**Definition 11 (Generalized Discrete Hamilton’s Principle (GDHP))**

Critical points of the discrete action

$$S^L_d = \sum_{k=0}^{n-1} \bar{L}_d(q^d_k, t^d_k, \Delta_q^d q^d_k, \Delta_t^d t^d_k) \tau, \quad (80)$$

in the class of discrete curves $(q^d_k, t^d_k)_k$ with endpoints $(\tau_0, t_0, q_0)$ and $(\tau_n, t_n, q_n)$ correspond to trajectories of the discrete Hamiltonian system going from $(t_0, q_0)$ to $(t_n, q_n)$:

Again, to proceed to the derivation of the equations of motion we need to specify the derivative operator.

### 5.1.3 Generalized discrete modified Hamilton’s principle

**Definition 12** Let $\bar{L}_d$ be a discrete Lagrangian on $T\mathcal{M}$ and define the discrete Legendre transform (or discrete fiber derivative) $FL : T\mathcal{M} \rightarrow T^*\mathcal{M}$ which maps the discrete extended phase space $T\mathcal{M}$ to $T^*\mathcal{M}$ by

$$(q^d_k, t^d_k, \Delta_q^d q^d_k, \Delta_t^d t^d_k) \mapsto (q^d_k, t^d_k, p^d_k, e^d_k), \quad (81)$$

where

$$p^d_k = \frac{\partial \bar{L}_d(q^d_k, t^d_k, \Delta_q^d q^d_k, \Delta_t^d t^d_k)}{\partial \Delta_q^d q^d_k}, \quad e^d_k = \frac{\partial \bar{L}_d(q^d_k, t^d_k, \Delta_q^d q^d_k, \Delta_t^d t^d_k)}{\partial \Delta_t^d t^d_k}. \quad (82)$$

The Legendre transform as defined by equations (82) is equivalent to the previous definition (equation (5)). Indeed,

$$\frac{\partial \bar{L}_d(q^d_k, t^d_k, \Delta_q^d q^d_k, \Delta_t^d t^d_k)}{\partial \Delta_q^d q^d_k} = \frac{\partial L_d(q^d_k, \Delta_q^d q^d_k)}{\partial \Delta_t^d t^d_k} = D_2 L_d(q^d_k, \Delta_q^d q^d_k),$$

where $\Delta_t^d = \frac{\Delta^d_t}{\Delta^d_t q^d_k}$ represent the discrete derivative with respect to time.

If the discrete fiber derivative is a local isomorphism, $\bar{L}_d$ is called regular and if it is a global isomorphism we say that $\bar{L}_d$ is hyperregular. If $\bar{L}_d$ is hyperregular,
we define the corresponding discrete Hamiltonian function on $T^*\mathcal{M}$ by
\[ \bar{H}_d(q_k^d, t_k^d, p_k^d, e_k^d) = \langle p_k^d, \Delta^d q_k^d \rangle - \bar{L}_d(q_k^d, \Delta^d q_k^d), \tag{83} \]
where $\Delta^d q_k$ is defined implicitly as a function of $(q_k^d, p_k^d)$ through equation (82). $\bar{H}_d$ is related to the previously defined Hamiltonian function by the following relationship:
\[ \bar{H}_d(q_k^d, t_k^d) = \Delta^d q_k^d \bar{H}_d(q_k^d, p_k^d). \tag{84} \]
In addition, we have: $e_k^d = -\bar{H}_d(q_k^d, p_k^d)$, that is, the momentum associated with the time is the opposite of the Hamiltonian.

Let $S^H_d$ be the discrete action summation:
\[ S^H_d = \tau \sum_{k=0}^{n-1} \langle p_k^d, \Delta^d q_k^d \rangle - \bar{H}_d(q_k^d, p_k^d) \]
\[ = \tau \sum_{k=0}^{n-1} \langle p_k^d, \Delta^d q_k^d \rangle + \langle e_k^d, \Delta^d t_k^d \rangle. \tag{85} \]

Before stating the generalized discrete modified Hamilton’s principle, we need to remark that all the coordinates are not independent since the holonomic constraint $e_k^d = -H(q_k^d, p_k^d)$ holds. There are two ways to handle this situation [3], one can either replace $e_k^d$ by $-H(q_k^d, p_k^d)$ in the action and then take the variations or one can use Lagrange multiplier to append the constraint $e_k^d + H(q_k^d, p_k^d) = 0$ to the integral. Therefore we can give two equivalent formulations of the GDMHP.

**Definition 13 (Generalized discrete modified Hamilton’s principle)**

*Critical points of the discrete action*

\[ S^H_d = \tau \sum_{k=0}^{n-1} \langle p_k^d, \Delta^d q_k^d \rangle + \langle e_k^d, \Delta^d t_k^d \rangle \]

in the class of discrete curves $(q_k^d, t_k^d, p_k^d, e_k^d)$ with endpoints $(\tau_0, t_0, q_0)$ and $(\tau_n, t_n, q_n)$ subject to the constraint $e_k^d + H_d(q_k^d, p_k^d) = 0$ correspond to discrete trajectories of the discrete Hamiltonian system going from $(t_0, q_0)$ to $(t_n, q_n)$.

**Definition 14 (Generalized discrete modified Hamilton’s principle)**

*Critical points of the discrete action*

\[ S^H_d = \tau \sum_{k=0}^{n-1} \langle p_k^d, \Delta^d q_k^d \rangle - \bar{H}_d(q_k^d, p_k^d) \Delta^d t_k^d \]

in the class of discrete curves $(q_k^d, t_k^d, p_k^d)$ with endpoints $(\tau_0, t_0, q_0)$ and $(\tau_n, t_n, q_n)$ correspond to discrete trajectories of the discrete Hamiltonian system going from $(t_0, q_0)$ to $(t_n, q_n)$. 

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To derive the equations of motion we need to specify the discrete derivative operator, \( \Delta^d \) and its associated Leibnitz law.

\section*{5.2 Examples}

\subsection*{5.2.1 Störmer type of algorithm}

\subsubsection*{5.2.1.1 Lagrangian approach}

Consider a Lagrangian function \( L(q, \dot{q}) \) and define the discrete Lagrangian map trivially by \( L_d(q_k, \Delta \tau q_k) = L(q_k, \Delta \tau q_k) \).

Discrete equations of motion are obtained from the generalized discrete Hamilton’s principle:

\[
\delta S_d^L = \tau \sum_{k=0}^{n-1} \delta L_d(q_k, t_k, \Delta \tau q_k, \Delta \tau t_k) \\
= \tau \sum_{k=0}^{n-1} \delta (\Delta \tau t_k L_d(q_k, \frac{\Delta \tau q_k}{\Delta \tau t_k})) \\
= \tau \sum_{k=0}^{n-1} (\delta \Delta \tau t_k)L_d^k + \Delta \tau t_k D_1 L_d^k \delta q_k \\
+ \Delta \tau t_k D_2 L_d^k \left( \frac{\Delta \tau \delta q_k}{\Delta \tau t_k} - \frac{\Delta \tau q_k}{(\Delta \tau t_k)^2} \delta \Delta \tau t_k \right),
\]

where \( L_d^k = L_d(q_k, \frac{\Delta \tau q_k}{\Delta \tau t_k}) \). Using the Leibnitz law (equation (1)) and the fixed end points constraint, we obtain:

\[
\delta S_d^L = \tau \sum_{k=1}^{n-1} -\Delta \tau e_{k-1} \delta t_k + (-\Delta \tau D_2 L_d^{k-1} + \Delta \tau t_k D_1 L_d^k) \delta q_k, \quad (87)
\]

where we have used the fixed end points constraint to derive the last equation and defined

\[
e_{k+1} = \frac{\partial L_d^k}{\partial \Delta \tau t_k} = L_d(q_k, \frac{\Delta \tau q_k}{\Delta \tau t_k}) - D_2 L_d(q_k, \frac{\Delta \tau q_k}{\Delta \tau t_k}) \frac{\Delta \tau q_k}{\Delta \tau t_k}.
\]

Finally we obtain the modified Euler-Lagrange equations by setting the variations to zero:

\[
e_k - e_{k-1} = 0,
\]

\[
\Delta \tau t_k D_1 L_d(q_k, \frac{\Delta \tau q_k}{\Delta \tau t_k}) - \Delta \tau D_2 L_d(q_{k-1}, \frac{\Delta \tau q_{k-1}}{\Delta \tau t_{k-1}}) = 0. \quad (88)
\]
Lemma 15 The algorithm defined by (88) preserves the Lagrangian two-form and the energy.

PROOF. The first equation of the algorithm proves energy conservation. To show that the Lagrangian two-form is preserved, we compute $dS_d^L$ along a discrete trajectory:

$$dS_d^L = \tau \sum_{k=1}^{n-1} \Delta_\tau (L_d^{k-1} dt_k) + \Delta_\tau (D_2 L_d^{k-1} dq_k) - \Delta_\tau \left( \frac{D_2 L_d^{k-1}}{\Delta_\tau t_{k-1}} \Delta_\tau q_{k-1} dt_k \right)$$

$$= \tau \sum_{k=1}^{n-1} \Delta_\tau (e_k dt_k + D_2 L_d^{k-1} dq_k)$$

$$= \tau \sum_{k=1}^{n-1} \Delta_\tau \theta_L^k ,$$

where $\theta_L^k = e_k dt_k + D_2 L_d^{k-1} dq_k$. Since $d^2 = 0$, we obtain that the symplectic two-form $\omega_L^k = d\theta_L^k$ is preserved along the trajectory.

The proof of this lemma only involves the modified Leibnitz law and does not depend on the definition of the discrete Lagrangian function. As a consequence, it also applies if one derives modified velocity Verlet and Newmark algorithms.

5.2.1.2 Hamiltonian approach Let the Lagrangian function be $L(q, \dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q)$. Then

$$\bar{L}_d = \Delta_\tau t_k \left( \frac{1}{2} \frac{\Delta_\tau q_k}{\Delta_\tau t_k} M \frac{\Delta_\tau q_k}{\Delta_\tau t_k} - V(q_k) \right),$$

and the associated momenta are:

$$p_{k+1} = M \frac{\Delta_\tau q_k}{\Delta_\tau t_k} ,$$

$$e_{k+1} = -\frac{1}{2} \frac{\Delta_\tau q_k}{\Delta_\tau t_k} M \frac{\Delta_\tau q_k}{\Delta_\tau t_k} - V(q_k).$$

The discrete Hamiltonian function is then:

$$\bar{H}_d = \Delta_\tau t_k \left( \frac{1}{2} p_{k+1}^T M^{-1} p_{k+1} + V(q_k) \right) = \Delta_\tau t_k H_d(q_k, p_{k+1}).$$

One can readily verify that $H_d(q_k, p_{k+1}) = -e_{k+1}$.
Let us now derive the modified discrete equations of motion by applying the GDMHP (theorem (14)). We skip a few steps in the evaluation of the variations of $S_d^H$ to finally find:

$$\delta S_d^H = \tau \delta \sum_{k=0}^{n-1} \langle p_{k+1}, \Delta_\tau q_k \rangle - \dot{H}_d(q_k, p_{k+1})$$

$$= \tau \sum_{k=0}^{n-1} \langle \Delta_\tau q_k - \Delta_\tau t_k D_2 H_d(q_k, p_{k+1}), \delta p_{k+1} \rangle$$

$$- \langle \Delta_\tau p_k + \Delta_\tau t_k D_1 H_d(q_k, p_{k+1}), \delta q_k \rangle + \Delta_\tau e_{k+1} \delta t_{k+1}.$$  

(93)

The variations of $(\delta q_k, \delta p_{k+1}, \delta t_k)$ being independent, we obtain:

$$\Delta_\tau q_k = \Delta_\tau t_k p_{k+1},$$

$$\Delta_\tau p_k = -\Delta_\tau t_k \nabla V(q_k),$$

$$\Delta_\tau e_k = 0.$$  

(94)

**Lemma 16** The algorithm defined by equations (94) preserves the symplectic two-form and the energy.

**PROOF.** The proof proceeds as the previous ones, we compute $dS_d^H$ along a discrete trajectory. We skip the detail of the computation:

$$dS_d^H = \tau \sum_{k=0}^{n-1} \Delta_\tau \langle p_k, dq_k \rangle + e_k dt_k.$$  

(95)

Define $\theta_k^H = \langle p_k, dq_k \rangle + e_k dt_k$ and $\omega_k^H = d\theta_k^H$. Since $d^2 = 0$, we obtain

$$\Delta_\tau \omega_k^H = 0.$$

**Remark 17** The 1-form $\theta_k^H$ corresponds to the contact 1-form $\theta$ encountered in continuous time dynamics. Indeed, if one remembers that $e_k = -H_d(q_{k-1}, p_k)$, then we have:

$$\theta = pdq - H dt,$$

$$\theta_k^H = p_k dq_k - H_d(q_{k-1}, p_k) dt_k.$$  

(96)  

(97)
5.2.2 Midpoint discretization

In the same manner, we can apply the modified variational principle to other discretization. For the midpoint scheme we have 
\[ q^d_k = \frac{q_{k+1} + q_k}{2} \] and the modified Leibnitz rule is defined by equation (46). Let us define the generalized momenta:

\[ p_k^{d+1} + p_k^d = \frac{\partial \bar{L}_d}{\partial \Delta^d_r q^d_k}, \quad (98) \]

\[ e_k^{d+1} + e_k^d = \frac{\partial \bar{L}_d}{\partial \Delta^d_r e^d_k}. \quad (99) \]

Then applying the modified discrete Hamilton’s principle (Definition (14)) yields (after a few simplifications):

\[ \delta S^H_d = \tau \sum_{k=0}^{n-1} \langle \Delta^d_r \tau_k D_1 L^d_k - \Delta^d_r \tau_k p^d_k, \delta q^d_k \rangle - \Delta^d_r \tau_k \delta t^d_k, \quad (100) \]

where \( L^d_k = L_d(q^d_k, \Delta^d_r q^d_t) \). The variations \( (\delta q^d_k, \delta t^d_k) \) being independent, we obtain:

\[ \frac{p_{k+1} - p_k}{\tau} = \frac{t_{k+1} - t_k}{\tau} D_1 L^d_k \left( \frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right), \]

\[ e_{k+1} = e_k, \]

\[ \frac{p_{k+1} + p_k}{2} = \frac{t_{k+1} - t_k}{\tau} D_2 L^d_k \left( \frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right), \]

\[ e_{k+1} + e_k = L_d \left( \frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right) \]

\[ - \langle D_2 L^d_k \left( \frac{q_{k+1} + q_k}{2}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right), \delta q^d_k \rangle, \quad (101) \]

Lemma 18 The algorithm defined by equations (101) preserves the Lagrangian two-form as well as the energy.

**PROOF.** We omit the proof since it proceeds as before.

Now define the discrete Hamiltonian function \( H_d(q^d_k, p^d_k) = H \left( \frac{q_{k+1} + q_k}{2}, \frac{p_{k+1} + p_k}{2} \right) \) and the modified Hamiltonian function \( \bar{H}_d = \Delta^d_r \tau_k H_d(q^d_k, p^d_k) \). Then applying the GDMHP yields:
\begin{align*}
\frac{q_{k+1} - q_k}{\tau} &= \frac{t_{k+1} - t_k}{\tau} D_2 H_d \left( \frac{q_{k+1} + q_k}{2}, \frac{p_{k+1} + p_k}{2} \right), \\
\frac{p_{k+1} - p_k}{\tau} &= -\frac{t_{k+1} - t_k}{\tau} D_1 H_d \left( \frac{q_{k+1} + q_k}{2}, \frac{p_{k+1} + p_k}{2} \right), \\
e_{k+1} - e_k &= 0, \\
e_{k+1} + e_k &= -H_d \left( \frac{q_{k+1} + q_k}{2}, \frac{p_{k+1} + p_k}{2} \right). 
\end{align*}
(102)

**Lemma 19** The algorithm defined by equations (102) preserves the symplectic two-form as well as the energy.

**PROOF.** We omit the proof since it proceeds as before.

### 5.3 Concluding remarks

The algorithm defined by equations (102) is the same as the one developed by Shibberu [32]. Shibberu’s approach corresponds to the first formulation of the GDMHP (definition (13)) for the midpoint rule but he used a different discrete variational principle from DVPII.

One other work on symplectic energy preserving algorithms is that of Kane, Marsden and Ortiz [23]. They developed a generalized discrete modified Hamilton’s principle that is based on DVPI. Their approach is different from ours: they assume a different time step at each iteration, and then take the variation of the discrete action without varying the time step (i.e., in a $n$ dimensional space). As a consequence they only obtain $n$ equations for the $n + 1$ variables $(q_k, h_k)$ where $h_k$ is the time step at the $k^{th}$ step. They then add an energy constraint to obtain $n + 1$ equations. Their definition of the energy is similar to ours and therefore both methods provide the same algorithms. However, there are fundamental differences between the two methods. First, the method developed in this paper is fully variational. Second, all the differences between DVPI and DVPII that we emphasize at the beginning of this paper still remain because their work is based on DVPI whereas our is based on DVPII.

### 6 Discrete Hamilton-Jacobi theory

So far we have developed two variational principles that are the discrete counterparts of Hamilton’s principle on the tangent bundle and on the cotangent bundle. Through several examples we have observed that both variational principles are equivalent and that they allow us to recover classical variational symplectic integrators. We have also shown that they can be modified so that
energy conservation is assured. In this section, we concentrate on discrete Hamilton-Jacobi theory. We define discrete canonical transformations (DCT), discrete generating functions (DGF) and derive a discrete Hamilton-Jacobi equation that allows us to show that the energy error for a certain class of scheme is invariant under discrete canonical transformations.

6.1 Discrete symplectic geometry

We consider again a discretization of the time $t$ into $n$ instants $\mathcal{T} = \{(t_k)_{k \in \{1,n\}}\}$ but we restrict here to the case where $M_k$ is a $n$-dimensional vector space. We still define $\mathcal{M} = \bigcup M_k$.

**Definition 20** A discrete symplectic form $\omega$ on $\mathcal{M}$ is such that at $t_k$, $\omega = \omega^d_k$, where $\omega^d_k$ is a non degenerate, closed, two-form on $M^d_k = M_k \cup M_{k+1}$. A discrete canonical one-form, $\theta$ on $\mathcal{M}$ is such that at $t_k$, $\theta = \theta^d_k$, and $\omega^d_k = -d\theta^d_k$. A discrete symplectic vector space $(\mathcal{M}, \omega)$ is a vector space $\mathcal{M} = \bigcup M_k$ together with a discrete symplectic two form on $\mathcal{M}$.

Using a symplectic chart, a discrete symplectic form on $\mathcal{M}$ at $t_k$ can be written as:

$$\omega^d_k = dq^d_k \wedge dp^d_k, \quad (103)$$

and the canonical one-form as $\theta^d_k = p^d_k dq^d_k$.

In the remainder of this section we consider the geometry associated with the midpoint scheme, that is, we define $z^d_k = (q^d_k, p^d_k)$ as $z^d_k = \frac{z_k + z_{k+1}}{2}$ and use the modified Leibnitz law (46). However, the content of this section can be applied to any scheme as long as one can define a discrete Hamiltonian vector field from the discrete Hamiltonian function and the discrete symplectic two-form (see next definition). It is clear that the theory herein can be adapted to systems for which the action integral involves a term of the form $H^d_d(z^d_k)$, where $z^d_k$ is a linear combination of $z_k$ and $z_{k+1}$ but it is not clear if it can be adapted to the Störmer rule for instance ($z^d = (q_k, p_{k+1})$ cannot be written as a linear combination of $z_{k+1}$ and $z_k$ so the next definition does not apply). We do not know how to modify this approach so that a discrete Hamiltonian vector field can be defined from the Hamiltonian function $H^d_d(q_k, p_{k+1})$.

**Definition 21** Let $(\mathcal{M}, \omega)$ be a discrete symplectic vector space, and $H^d : \mathcal{M} \to \mathbb{R}$ a smooth function. Define the discrete vector field $X^d_H$ such that at $t_k$, $X^d_H = X^d_k$, where $X^d_k$ is of the form

$$X^d_H = \Delta^d q^d_k \frac{\partial}{\partial q^d_k} + \Delta^d p^d_k \frac{\partial}{\partial p^d_k}, \quad (104)$$
and verifies:

\[ i_{X^d_k} \omega^d_k = dH_d. \]  

(105)

The discrete vector field \( X^d_H \) is called the discrete Hamiltonian vector field. 
\((\mathcal{M}, \omega, X^d_H)\) is called a discrete Hamiltonian system.

**Proposition 22** Using the canonical coordinates, a Hamiltonian vector field is of the form:

\[ X^d_H = J \cdot dH_d, \]  

(106)

where \( J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \).

**PROOF.** Equation (105) is expressed in local coordinates as:

\[ i_{X^d_H} (dq_k^d \wedge dp_k^d) = D_1 H_d(z_k^d) dq_k^d + D_2 H_d(z_k^d) dp_k^d. \]  

(107)

Let \( X^d_H \) be:

\[ X^d_H = \Delta^d_{q_k^d} \frac{\partial}{\partial q_k^d} + \Delta^d_{p_k^d} \frac{\partial}{\partial p_k^d}, \]  

(108)

then,

\[ i_{X^d_H} (dq_k^d \wedge dp_k^d) = (i_{X^d_H} dq_k^d) dp_k^d - dq_k^d \wedge (i_{X^d_H} dp_k^d) \]  

(109)

\[ = \Delta^d_{p_k^d} dq_k^d - \Delta^d_{q_k^d} dp_k^d. \]  

(110)

Identifying this last equation with equation (107) leads to equation (106).

### 6.2 Discrete canonical transformation

We now define the class of discrete canonical transformations. The definition given here is restricted to linear time-dependent maps (with respect to the phase space variables). We believe larger class of transformations may be considered if one works with discretization of the spacetime [25]. Let \((\mathcal{M}_1, \omega_1)\) and \((\mathcal{M}_2, \omega_2)\) be discrete symplectic vector spaces and \( \mathcal{F} \) be the set maps \( f : \mathcal{T} \times \mathcal{M}_1 \to \mathcal{T} \times \mathcal{M}_2 \) that are linear with respect to the phase space variables. Consider a map \( f \in \mathcal{F} \) such that \( \forall t_k \in \mathcal{T}, f(t_k, \cdot) = f_k(\cdot) \) where \( f_k \) is the following linear map:

\[ M_{1,k}^d \to M_{2,k}^d \]

\[ z_k = (q_k, p_k) \mapsto Z_k = (Q_k, P_k) = A_k z_k + B_k. \]
Since $f_k$ is linear, we have:

$$f_k(z^d_k) = \frac{1}{2}(f_k(z_k) + f_k(z_{k+1})),$$  \hspace{1cm} (111)

$$f_k(\Delta^d_z, z^d_k) = A_k \Delta^d_z z^d_k.$$  \hspace{1cm} (112)

**Definition 23** A linear, time-dependent map $f$ is called a discrete canonical transformation (DCT) (or a discrete symplectic map) if and only if $f^* \omega_2 = \omega_1$, or equivalently, $\forall k \in [1, n], f_k^* \omega_{2,k} = \omega_{1,k}$.

**Proposition 24** If $f$ is a DCT then $A_k$ is invertible for all $k \in [1, n]$

**PROOF.** Suppose there exists a $k$ such that $A_k$ is not invertible. Then $\exists z^d_k \in M^d_{1,k}$ such that $\exists v_1 \in T_{z^d_k}M^d_{1,k} | T f_k \cdot v_1 = 0.$

Then, $\forall v_2 \in T_{z^d_k}M^d_{1,k} | v_2 \neq 0$, $\omega^d_{1,k}(v_1, v_2) = \omega^d_{2,k}(T f_k \cdot v_1, T f_k \cdot v_2)$ since $f$ is symplectic. The right hand side is zero but the left hand side is not. This is a contradiction and therefore $A_k$ is invertible.

**Lemma 25** Let $f$ be a discrete canonical transformation. Then $f^*_k \omega^d_{2,k} = \omega^d_{1,k}$ can be written in the matrix form $A_k J A^T_k = J$. In addition, $f$ preserves the form of the discrete Hamilton’s equations.

**PROOF.** The statement $A_k J A^T_k = J$ is just the matrix statement of $f^*_k \omega^d_{2,k} = \omega^d_{1,k}$. Let us prove that $f$ preserves the form of the discrete Hamilton’s equations. Define the function $K_d$ such that $K_d \circ f = H_d$.

On one hand, using equation (112) we have:

$$\Delta^d_z Z^d_k = \frac{f_k(z_{k+1}) - f_k(z_k)}{\tau} = A_k \Delta^d_z z^d_k.$$  \hspace{1cm} (113)

On the other hand:

$$J \nabla H_d(z^d_k) = J \nabla (K_d \circ f_k(z^d_k)) = J A^T_k \nabla K_d(z^d_k).$$  \hspace{1cm} (115)

Since $A_k J A^T_k = J$, we obtain:

$$\Delta^d_z Z^d_k = J \nabla K_d(z^d_k)$$  \hspace{1cm} (117)
This last result can be summarized as follows:

**Proposition 26** Let $X^d_H$ be a discrete Hamiltonian vector field with Hamiltonian function $H_d$ and $f$ a discrete symplectic map. Then $f_* X^d_H$ is a discrete Hamiltonian vector field with Hamiltonian function $f_* H_d$.

### 6.3 Discrete generating functions

**Proposition 27** Let $(\mathcal{M}_1, \omega_1)$ and $(\mathcal{M}_2, \omega_2)$ be two discrete symplectic vector spaces, $\pi_i : \mathcal{M}_1 \times \mathcal{M}_2 \to \mathcal{M}_i$ the projection onto $\mathcal{M}_i$ and define

$$\Omega = \pi_1^\ast \omega_1 - \pi_2^\ast \omega_2.$$  \hspace{1cm} (118)

Then,

1. $\Omega$ is a discrete symplectic form on $\mathcal{M}_1 \times \mathcal{M}_2$,
2. a map $f : \mathcal{M}_1 \to \mathcal{M}_2$ is a discrete symplectic map if and only if $i_f^\ast \Omega = 0$, where $i_f : \Gamma_f \to \mathcal{M}_1 \times \mathcal{M}_2$ is the inclusion map and $\Gamma_f$ is the graph of $f$.

**Proof.** We recall that at $t_k$, $\Omega = \Omega_k^d$ where $\Omega_k^d = \pi_1^\ast \omega_{1,k}^d - \pi_2^\ast \omega_{2,k}^d$. To prove that $\Omega$ is a discrete symplectic form, we need to prove that $\Omega_k^d$ is a symplectic form on $\mathcal{M}_1 \times \mathcal{M}_2$ for all $k \in [1, n]$.

\[
\begin{align*}
    d\Omega_k^d &= d(\pi_1^\ast \omega_{1,k}^d - \pi_2^\ast \omega_{2,k}^d) \\
    &= \pi_1^\ast d\omega_{1,k}^d - \pi_2^\ast d\omega_{2,k}^d \\
    &= 0,
\end{align*}
\]

since $\omega_{i,k}^d$ is closed and $d$ commutes with the pull back operator.

Now let $z_k^d = (z_{1,k}^d, z_{2,k}^d) \in \mathcal{M}_{1,k}^d \times \mathcal{M}_{2,k}^d$ and $v = (v_1, v_2) \in T_{z_k^d}^d (\mathcal{M}_{1,k}^d \times \mathcal{M}_{2,k}^d) \sim T_{z_{1,k}^d}^d \mathcal{M}_{1,k}^d \times T_{z_{2,k}^d}^d \mathcal{M}_{2,k}^d$ such that

$$\forall w = (w_1, w_2) \in T_{z_k^d}^d (\mathcal{M}_{1,k}^d \times \mathcal{M}_{2,k}^d) \quad \Omega_k^d(v, w) = 0$$  \hspace{1cm} (122)

and let us prove that $v$ is zero. We have

\[
\begin{align*}
    \Omega_k^d(v, w) &= \omega_{1,k}^d(\pi_1(z_{1,k}^d)(T\pi_1 \cdot v, T\pi_1 \cdot w) - \omega_{2,k}^d(\pi_2(z_{2,k}^d)(T\pi_2 \cdot v, T\pi_2 \cdot w) \\
    &= \omega_{1,k}^d(z_{1,k}^d)(v_1, w_1) - \omega_{2,k}^d(z_{2,k}^d)(v_2, w_2)
\end{align*}
\]

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The right hand side of equation (124) is zero for all \( w \) if and only if both terms are zero, that is,
\[
\omega^d_{1,k}(z^d_{1,k})(v_1, w_1) = 0, \quad \omega^d_{2,k}(z^d_{2,k})(v_2, w_2) = 0
\]  
(125)

Since \( \omega^d_{i,k} \) is non degenerate, \( v_1 = v_2 = 0 \) and \( \Omega^d_k \) is closed.

We now prove the second statement of the proposition. We first notice that \( f_k \) induces a diffeomorphism of \( M^d_{i,k} \) to \( \Gamma_{f_k} \), so we can write
\[
T_{(z^d_{i,k}, f_k(z^d_{i,k}))} = \left\{(v, T f_k \cdot v) \mid v \in T_{z^d_{i,k}} M^d_{i,k}\right\}
\]
(126)

Then,
\[
i^*\Omega^d_k((v_1, T f_k \cdot v_1), (v_2, T f_k \cdot v_2)) = \omega^d_{1,k}(v_1, v_2) - \omega^d_{1,k}(T f_k \cdot v_1, T f_k \cdot v_2)
= (\omega^d_{1,k} - f_k^*\omega^d_{2,k})(v_1, v_2)
\]
(127)

Hence, \( f_k \) is symplectic if and only if \( i^*\Omega^d_k = 0 \), i.e., \( f \) is a discrete symplectic map if and only if \( i^*\Omega = 0 \).

Using the Poincaré lemma we may write \( \Omega^d_k = -d\Theta^d_k \) and the previous proposition says that \( i^*_f \Theta^d_k \) is closed if and only if \( f \) is a discrete symplectic map.

Using again the Poincaré lemma, we conclude that if \( f \) is a discrete symplectic map then there exists a function \( S : \Gamma_f \to \mathbb{R} \) such that \( i^*_f \Theta = dS \), i.e., \( \forall k \in [1, n], i^*_f \Theta^d_k = dS_k \).

**Definition 28** Such a function \( S \) is called a discrete generating function for the discrete symplectic map \( f \). \( S \) is locally defined and depends on the choice of \( \Theta \).

- Let \( \theta^d_{1,k} = p^d_k dq^d_k \) and \( \theta^d_{2,k} = P^d_k dQ^d_k \), then
  \[
  i^*_f \Theta^d_k = (\pi_1 \circ i_f)^* p^d_k dq^d_k - (\pi_2 \circ i_f)^* P^d_k dQ^d_k, \quad \frac{dS}{dq}(q^d_k, Q^d_k) dq^d_k + \frac{dS}{dQ}(q^d_k, Q^d_k) dQ^d_k, \quad \frac{dS}{dQ}(q^d_k, Q^d_k).
  \]
(128)

  that is,
  \[
p^d_k = \frac{dS}{dq}(q^d_k, Q^d_k) \quad P^d_k = -\frac{dS}{dQ}(q^d_k, Q^d_k).
  \]
(130)

\( S \) as defined corresponds to a discrete generating function of the first kind.

- Let \( \theta^d_{1,k} = p^d_k dq^d_k \) and \( \theta^d_{2,k} = -Q^d_k dP^d_k \), then
  \[
i^*_f \Theta^d_k = (\pi_1 \circ i_f)^* p^d_k dq^d_k + (\pi_2 \circ i_f)^* Q^d_k dP^d_k, \quad \frac{dS}{dq}(q^d_k, Q^d_k) dq^d_k + \frac{dS}{dQ}(q^d_k, Q^d_k) dQ^d_k.
  \]
(131)
that is,
\[
\begin{align*}
\mathcal{P}_d^k &= \frac{\partial S}{\partial q_k}(q^d_k, Q^d_k) & \mathcal{Q}_d^k &= \frac{\partial S}{\partial P_k}(q^d_k, P^d_k).
\end{align*}
\] (133)

\(S\) as defined corresponds to a discrete generating function of the second kind.

In the same way, one can define \(4^n\) generating functions as in the continuous case. Note that since \(f\) is linear with respect to its spatial variables, \(S\) is also linear with respect to its spatial variables. At \(t_k\), \(S = S_k\) where \(S_k(\cdot) = T_k(\cdot) + U_k\) is affine map, \(T_k\) is a \(2n \times 2n\) matrix and \(U_k\) is a \(2n \times 1\) matrix.

6.4 Discrete Hamilton-Jacobi theory

In this section we use the notions introduced previously to develop a discrete Hamilton-Jacobi theory. Let \(f\) be a discrete symplectic map, let \(M_{i,k}^d = T^*Q_{i,k}^d\) and let \(S\) be an associated discrete generating function such that at \(t_k\), \(S = S_k\) where

\[
S_k(\cdot) = T_k(\cdot) + U_k
\]

Theorem 29 Define
\[
\begin{align*}
\mathcal{P}_d^d(q^d_k, Q^d_k) &= D_1S_k(q^d_k, Q^d_k), & \mathcal{Q}_d^d(q^d_k, Q^d_k) &= -D_2S_k(q^d_k, Q^d_k).
\end{align*}
\]

Then the following two conditions are equivalent:

(1) \(S\) is a discrete generating function associated with \(f\);
(2) For every curve \((c_k)_k\) in \(Q_1 = \bigcup Q_{1,k}\) satisfying:
\[
\Delta^d_t c_k = T_{\pi^*_Q_{1,k}} X^d_H(c_k, \mathcal{P}_k),
\] (134)
the curve \(k \mapsto (c_k^d, \mathcal{P}_k^d)\) is a discrete integral curve of \(X^d_H\), where \(\pi^*_Q_{1,k}\) is the cotangent bundle projection onto the configuration space.

For every curve \((c_k)_k\) in \(Q_2 = \bigcup Q_{2,k}\) satisfying:
\[
\Delta^d_t c_k = T_{\pi^*_Q_{2,k}} X^d_K(c_k, \mathcal{P}_k),
\] (135)
the curve \(k \mapsto (c_k^d, \mathcal{P}_k^d)\) is a discrete integral curve of \(X^d_K\), where \(\pi^*_Q_{2,k}\) is the cotangent bundle projection onto the configuration space.

**Proof.** Suppose \(S\) is a discrete generating function, let \(Q_k^d\) be fixed and consider a curve \((c_k)_k\) verifying
\[
\Delta^d_t c_k = T_{\pi^*_Q_{1,k}} X^d_H(c_k, \mathcal{P}_k),
\] (136)
In other words, \( c_k \) verifies:

\[
\Delta^d\tau^d c_k = D_2 H(c_k, \tilde{p}_k^d),
\]

(137)

Since \( S \) is a generating function, \( \tilde{p}_k^d \) is the momentum associated with \( c_k^d \) and verifies:

\[
\Delta^d\tilde{p}_k^d = -D_1 H(c_k, \tilde{p}_k^d).
\]

(138)

These last two equations are exactly a restatement of: \( k \mapsto (c_k^d, \tilde{p}_k^d) \) is a discrete integral curve of \( X^d_H \). To derive the second item we proceed in the same manner, but this time \( q_k^d \) is fixed.

Now we suppose item (2) and we show that \( S \) is a discrete generating function for \( f \). The statements \( k \mapsto (c_k^d, \tilde{p}_k^d) \) is a discrete integral curve of \( X^d_H \) and \( k \mapsto (c_k^d, \tilde{p}_k^d) \) is a discrete integral curve of \( X^d_K \) are equivalent to saying that \( \tilde{p}_k^d \) and \( \tilde{p}_k^d \) are the momenta associated with the generalized coordinates, and therefore, \( S \) is a generating function for \( f \).

**Theorem 30** We consider again a time dependent function \( S \) which is linear with respect to the spatial variables. Then the following two statements are equivalent:

1. \( S \) is a discrete generating function associated with \( f \);
2. For every \( H \) there is a function \( K \) such that

\[
H(q_k^d, D_1 S(q_k^d, Q_k^d)) = K(Q_k^d, D_2 S(q_k^d, Q_k^d))
\]

(139)

**PROOF.** Suppose \( S \) is a discrete generating function. Then from the previous theorem, for every curve \((c_k, C_k)\) in \( Q \times Q_2 \) satisfying \( \Delta^d c_k = T \pi^*_{Q_{1,k}} X^d_H(c_k, \tilde{p}_k) \) and \( \Delta^d C_k = T \pi^*_{Q_{2,k}} X^d_K(C_k, \tilde{p}_k) \), the curves \( k \mapsto (c_k, \tilde{p}_k) \) and \( k \mapsto (C_k, \tilde{p}_k) \) are discrete integral curves of \( X^d_H \) and \( X^d_K \) respectively. Then, using the symplectic identity ([1] page 382) that holds for any function \( S \)

\[
\omega^d_{1,k}(T(D_1 S \circ \pi^*_{Q_{1,k}}) \cdot v, w) = \omega^d_{1,k}(v, w - T(D_1 S \circ \pi^*_{Q_{1,k}}) \cdot w)
\]

we get:

\[
\omega^d_{1,k}(T(D_1 S \circ \pi^*_{Q_{1,k}}) \cdot X^d_H(c_k, D_1 S_k), w) =
\omega^d_{1,k}(X^d_H(c_k, D_1 S_k), w) - dH_d(c_k, D_1 S_k) \cdot TD_1 S(c_k, D_1 S_k) \cdot w
\]

(140)

\[
\omega^d_{2,k}(T(-D_2 S \circ \pi^*_{Q_{2,k}}) \cdot X^d_K(C_k, -D_2 S_k), w) =
\omega^d_{2,k}(X^d_K(C_k, -D_2 S_k), w) - dK_d(C_k, -D_2 S_k) \cdot TD_2 S(C_k, -D_2 S_k) \cdot w
\]

(141)
In addition, since \( p^d_k = D_1S(c^d_k, C^d_k) \) and \( P^d_k = -D_1S(c^d_k, C^d_k) \),

\[
\Delta^d v^d p^d_k = T D_1S(c^d_k, C^d_k) \Delta^d v^d c^d_k = T(D_1S \circ \pi^*_q D^1_k) \cdot X^d_H(c_k, D_1 S_k) \tag{142}
\]

\[
\Delta^d v^d P^d_k = T(-D_2S \circ \pi^*_q D^2_k) \cdot X^d_K(C_k, -D_2 S_k) \tag{143}
\]

\( f \) being a discrete canonical map, \( T f_k(\Delta^d v^d p^d_k) = \Delta^d v^d P^d_k \) so the left hand side of equation 141 is the image under \( f \) of the left hand side of (141). Using proposition (26), we conclude that:

\[
T f_k \cdot dH_d(c_k, D_1 S_k) \cdot T D_1S(c_k, D_1 S_k) = -dK_d(C_k, -D_2 S_k) \cdot T D_2 S(C_k, -D_2 S_k),
\]

which is equivalent to the discrete Hamilton-Jacobi equation.

The proof that 2. implies 1. follows from these arguments.

6.5 Applications of the discrete Hamilton-Jacobi theory

The goal of this section is to highlight the benefit of having a discrete Hamilton-Jacobi theory. First, we have proven the invariance of the discrete Hamilton’s equations under a certain class of coordinate transformations. Second, we have shown in theorem 30 that changing coordinates using a discrete symplectic map does not improve the performance of the algorithm in terms of energy conservation. As a consequence we have the following lemma:

**Lemma 31** The midpoint scheme preserves the energy for linear systems.

**PROOF.** The discrete phase flow for linear systems is piecewise linear continuous and the map \( (q_k, p_k) \mapsto (q_{k+1}, p_{k+1}) \) is symplectic (the midpoint scheme is a symplectic algorithm). Therefore, the discrete phase flow is a discrete symplectic map that maps \( H \) into a constant \( K \). Integration of the new Hamiltonian system defined by \( K \) is trivial \( ((Q_{k+1}, P_{k+1}) = (Q_k, P_k)) \) and obviously preserves the energy. As a consequence the integration of the Hamiltonian system defined by \( H \) also preserves the energy.

Finally, we illustrate the use of the above material with a nonlinear example. We study the energy error in the integration of the equations of motion of a particle in a double well potential using different sets of canonical coordinates. Consider a particle in a double well potential, i.e., \( H = \frac{1}{2}p^2 + \frac{1}{2}(q^4 - q^2) \).

As shown in figure (2), the midpoint scheme does not preserve the energy. The following time-dependent discrete canonical transformation (at each step the transformation is a different expression) \( Z_k = A_k z_k + B_k \) where \( A_k = \ldots \)
\[
\begin{pmatrix}
\cos(k\theta) - \sin(k\theta) \\
\sin(k\theta) \cos(k\theta)
\end{pmatrix},
\] and \(B_k = 0\) rotates the system by \(k\theta = k \arccos 0.99\) at the \(k^{th}\) step. In figure (3) we plot the same trajectory in the new system of coordinates, the energy error is exactly the same. In other words, the energy error is invariant under discrete canonical maps.

Fig. 2. Particle in a double well potential with initial conditions \((q, p) = (1, 0.05)\)

Fig. 3. Particle in the Hamiltonian vector field \(f^*X^d_H\), where \(X^d_H\) is the Hamiltonian vector field corresponding to a double well potential. Initial conditions are \((Q, P) = f_0(1, 0.05)\).

7 Optimal control

For a general optimal control problem, necessary conditions for optimality may be derived from the Pontryagin maximum principle. These conditions often yield equations of the same form as Hamilton’s equations coupled with
nonlinear equations. We have seen previously that Hamiltonian systems, i.e., Hamilton’s equations, can be integrated using symplectic integrators. However, if Hamilton’s equations are coupled with algebraic nonlinear equations, the above theory does not apply. What is the correct discretization of the algebraic equation? In this section, we develop a discrete maximum principle that tackles this problem and provides a unified view on solving optimal control problems using symplectic integrators.

7.1 Necessary conditions for optimality

7.1.1 Problem Statement

Let \( J = \int_0^T g(x, u)dt \) be a performance index (also called a cost function) and consider the following optimal control problem:

\[
\begin{align*}
\min_u \int_{t_0}^{t_f} g(x, u)dt, \\
\dot{x} &= f(x, u), \\
\phi_i(x(t_0), t_0) &= 0, \phi_f(x(t_f), t_f) = 0,
\end{align*}
\]

subject to the dynamics

\[\dot{x} = f(x, u),\]

and to the initial and final time constraints:

\[\phi_i(x(t_0), t_0) = 0, \phi_f(x(t_f), t_f) = 0,\]

where \( f \) and \( g \) are functions from \( \mathbb{R}^n \times \mathbb{R}^m \) to \( \mathbb{R} \) of class \( C^1 \).

7.2 Maximum principle

To solve the optimal control problem, we apply the maximum principle.

**Theorem 32 (Maximum principle)** Solutions to the optimal control problem defined by equations (144), (145) and (146) correspond to critical points of the cost function \( J \) in the class of curves \( \gamma = (x(t), u(t)) \in \Gamma \) where \( \Gamma \) is the set of curves satisfying (145) and (146).

**Remark 33** This formulation differs from the one given by Pontryagin [30] but the main point of the Pontryagin maximum principle is that it yields necessary conditions for optimality under far less severe regularity conditions. The above formulation is based on the equivalence between the Pontryagin maximum principle and the calculus of variations in the case where the control region is an open set in a finite dimensional vector space (see [30] chapter V
for more details). It is therefore equivalent to classical variational formulations given in Bloch et al. [3,4] and Gregory and Lin [11] for instance.

To apply the maximum principle we first need to define the augmented cost function $J_a$:

$$J_a = \int_{t_0}^{t_f} g(x, u) + \langle p, \dot{x} - f(x, u) \rangle \, dt + \langle \lambda_i, \phi_i(x(t_0), t_0) \rangle + \langle \lambda_f, \phi_f(x(t_f), t_f) \rangle$$

$$= \int_0^T H(x, p, u) - \langle p, \dot{x} \rangle \, dt + \langle \lambda_i, \phi_i(x(t_0), t_0) \rangle + \langle \lambda_f, \phi_f(x(t_f), t_f) \rangle,$$

where the $p$'s, the $\lambda_i$'s and the $\lambda_f$'s are Lagrange multipliers and $H(x, p, u) = g(x, u) + \langle p, f(x, u) \rangle$. Taking variations of the augmented cost function assuming fixed initial and final time yields:

$$\delta J_a = \delta \left( \int_{t_0}^{t_f} H(x, p, u) + \langle p, \dot{x} \rangle \, dt \right) + \delta \langle \lambda_i, \phi_i(x(t_0), t_0) \rangle$$

$$+ \delta \langle \lambda_f, \phi_f(x(t_f), t_f) \rangle$$

$$= \int_{t_0}^{t_f} \left( D_2 H(x, p, u) - \dot{x}, \delta p \right) + \left( D_1 H(x, p, u) + \dot{p}, \delta x \right)$$

$$+ \left( D_3 H(x, p, u), \delta u \right) \, dt + \langle -p(t_f) + D_1 \phi_f^T \lambda_f, \delta x_f \rangle$$

$$+ \langle p(t_i) + D_1 \phi_i^T \lambda_i, \delta x_i \rangle.$$

We now let the variations of $J_a$ be zero to obtain necessary conditions for optimality:

$$\dot{x} = D_2 H(x, p, u),$$

$$\dot{p} = -D_1 H(x, p, u),$$

$$0 = D_3 H(x, p, u),$$

as well as transversality conditions:

$$p(t_i) = -D_1 \phi_i(x(t_0), t_0)^T \lambda_i, \quad p(t_f) = D_1 \phi_f(x(t_f), t_f)^T \lambda_f.$$

Equations (147)-(150) define the necessary conditions for optimality.

### 7.3 Solving the necessary conditions for optimality

To solve these conditions, the most common technique is to find the optimal control feedback law from (149) and then use a shooting method to solve the two-point boundary value problem defined by (147), (148) and (150). More
precisely, suppose (149) allows one to solve for \( u \) as a function of \((x, p)\) and define the Hamiltonian function
\[
\bar{H}(x, p) = H(x, p, u(x, p)),
\]
then the necessary conditions (147) and (148) simplify to:
\[
\begin{align*}
\dot{x} &= D_2 \bar{H}(x, p), \quad (152) \\
\dot{p} &= -D_1 \bar{H}(x, p). \quad (153)
\end{align*}
\]
Equations (152) and (153) define a Hamiltonian system that has no physical meaning in general. As we will see later, for sub-Riemannian optimal control problems the Legendre transform is ill-defined and therefore DVPI cannot be used to discretize such systems whereas one could use DVPII (theorem 3). However, one may not be able to solve (149), and then the question of how one can use symplectic integrators to solve the optimal control problem arises. What is the correct discretization of (149)? In the next section we address this issue. Specifically, we introduce a discrete maximum principle that allows us to derive discrete necessary conditions for optimality that are in agreement with the one obtained from the maximum principle.

7.4 Discrete maximum principle

7.4.1 Problem statement

In discrete settings, the cost function is
\[
J = \sum_{k=0}^{n-1} g_d(x_k^d, u_k^d) \tau,
\]
and the optimal control problem (144) is formulated as:
\[
\min_{u_k^d} \sum_{k=0}^{n-1} g_d(x_k^d, u_k^d) \tau, \quad (154)
\]
subject to the dynamics
\[
\Delta^d x_k^d = f_d(x_k^d, u_k^d), \quad (155)
\]
and to boundary conditions:
\[
\phi_0(x_0, t_0) = 0, \quad \phi_n(x_n, t_n) = 0, \quad (156)
\]
where \( f_d \) and \( g_d \) are functions from \( \mathbb{R}^n \times \mathbb{R}^m \) to \( \mathbb{R} \) of class \( C^1 \). They correspond to discretization of the continuous time functions \( f \) and \( g \).
7.4.2 Discrete maximum principle

To obtain necessary conditions for optimality, we define the following discrete maximum principle, the discrete counterpart of the maximum principle:

**Definition 34 (Discrete maximum principle)** Solutions to the discrete optimal control problem correspond to critical points of the cost function \( J \) in the class of discrete curves \( \gamma \in \Gamma \), where \( \Gamma \) is the set of all discrete curves \((x_k, u_k)_{k \in [1,n]}\) that verify (155) and (156).

**Remark 35** The above definition is the discrete counterpart of the maximum principle. It compares to previous works on discrete optimal control theory that extend the Pontryagin maximum principle to discrete systems such as Jordan and Polak [22] as theorem 32 compares to the Pontryagin maximum principle. In other words, in contrast with Jordan and Polak [22], we restrict the class of discrete optimal control problems so that we can derive necessary conditions that define symplectic algorithms.

As in the continuous case, to find critical points of \( J \) under the non-holonomic constraint defined by equation (155), we must append the constraints to \( J \) using the Lagrange multipliers. The resulting function is called the augmented cost function:

\[
J_a = \sum_{k=0}^{n-1} (g_d(x^d_k, u^d_k) - \langle p^d_k, \Delta^d \tau x^d_k - f_d(x^d_k, u^d_k) \rangle) \tau + \langle \lambda_0, \phi_0 \rangle + \langle \lambda_n, \phi_n \rangle \tag{157}
\]

\[
= \sum_{k=0}^{n-1} (H_d(x^d_k, p^d_k, u^d_k) - \langle p^d_k, \Delta^d \tau x^d_k \rangle) \tau + \langle \lambda_0, \phi_0 \rangle + \langle \lambda_n, \phi_n \rangle, \tag{158}
\]

where the \( p_k \)'s, the \( \lambda_0 \)'s and the \( \lambda_n \)'s are Lagrange multipliers and \( H_d(x^d_k, p^d_k, u^d_k) = g_d(x^d_k, u^d_k) + \langle p^d_k, f_d(x^d_k, u^d_k) \rangle \). To apply the discrete maximum principle, one needs to specify the discrete derivative operator as well as the expressions of \( x^d_k, u^d_k \) and \( p^d_k \) as a function of \((x_{k+1}, x_k), (u_{k+1}, u_k)\) and \((p_{k+1}, p_k)\) respectively.

7.4.3 Examples

**7.4.3.1 Störmer’s rule** If we choose \( \Delta^d \) to be the forward difference \( \Delta \tau \) and \((x^d_k, p^d_k, u^d_k) = (x_k, p_{k+1}, u_k)\) then we recover the discrete maximum principle developed by Bloch, Crouch, Marsden and Ratiu [5].
\[ \delta J_a = \delta \left( \sum_{k=0}^{n-1} (H_d(x_k, p_k, u_k) + \langle p_k, \Delta^d x_k \rangle \tau) \right) + \delta \langle \lambda_0, \phi_0 \rangle + \delta \langle \lambda_n, \phi_n \rangle \]
\[ = \sum_{k=0}^{n-1} (D_2 H_d(x_k, p_{k+1}, u_k) - \Delta \tau x_k, \delta p_{k+1}) \tau \]
\[ + \langle D_1 H_d(x_k, p_{k+1}, u_k) + \Delta \tau p_k, \delta x_k \rangle \tau (+D_3 H_d(x_k, p_{k+1}, u_k), \delta u_k) \tau \]
\[ + \langle \phi_0, \delta \lambda_0 \rangle + \langle \phi_n, \delta \lambda_n \rangle + \langle -p_n + D_1 \phi^T_n \lambda_n, \delta x_n \rangle + \langle p_0 + D_1 \phi^T_0 \lambda_0, \delta x_0 \rangle , \]
(159)

where the modified Leibnitz law (1) has been used. We impose the variation of the augmented cost function to be zero to obtain discrete necessary conditions for optimality and transversality conditions:

\[ \Delta \tau x_k = D_2 H_d(x_k, p_{k+1}, u_k) , \quad \Delta \tau p_k = -D_1 H_d(x_k, p_{k+1}, u_k) , \]
\[ 0 = D_3 H_d(x_k, p_{k+1}, u_k) , \]
\[ p_0 = -D_1 \phi_0(x_0, t_0)^T \lambda_0 , \quad p_n = D_1 \phi_n(x_n, t_n)^T \lambda_n . \]

(160) (161) (162)

The algorithm defined by (160), (161) and (162) is equivalent to the one derived by Bloch, Crouch, Marsden and Ratiu [5] for the symmetric rigid body.

Lemma 36 The algorithm defined by (160), (161) and (162) is symplectic.

**Proof.** Define the cost function \( J_a \) as:

\[ \bar{J}_a = \sum_{k=0}^{n-1} (H_d(x_k, p_{k+1}, u_k) + \langle p_{k+1}, \Delta \tau x_k \rangle \tau) . \]

(164)

\( \bar{J}_a \) is the augmented cost function from which we have removed the boundary conditions. Boundary conditions yield transversality conditions, that is conditions on the initial and final states of the system. Hence these terms are irrelevant to the study of the advance map \( (x_k, p_k, u_k) \mapsto (x_{k+1}, p_{k+1}, u_{k+1}) \).

As in discrete dynamics, we consider \( d^2 \bar{J}_a \), assuming \( (x_k, p_k, u_k) \) verifies the above necessary conditions and we obtain:

\[ d \bar{J}_a = \sum_{k=0}^{n-1} \Delta \tau \langle p_k, dx_k \rangle \tau . \]

(165)

From \( d^2 = 0 \), we conclude:

\[ 0 = \sum_{k=0}^{n-1} \Delta \tau d \langle p_k, dx_k \rangle \tau , \quad \text{that is}, \quad \forall k \in [0, n-1] , \quad dp_{k+1} \wedge dx_{k+1} = dp_k \wedge dx_k . \]

(166)
The symplectic nature of the algorithm is obtained directly from the variational principle - there is no need to compute \( dp_k \wedge dx_k \) and \( dp_{k+1} \wedge dx_{k+1} \).

### 7.4.3.2 Midpoint scheme

Midpoint discretization may also be obtained if we choose

\[
\begin{align*}
    x^d_k &= \frac{x_{k+1} + x_k}{2}, \quad p^d_k = \frac{p_{k+1} + p_k}{2}, \quad u^d_k = \frac{u_{k+1} + u_k}{2}.
\end{align*}
\]

and \( \Delta^d_\tau = R_{\tau/2} - R_{-\tau/2} \). One can readily verify that the discrete maximum principle yields the following necessary conditions for optimality and transversality conditions:

\[
\begin{align}
    \Delta^d_\tau x^d_k &= D^2 H_d(x^d_k, p^d_k, u^d_k), \quad \text{(167)}
    \\
    \Delta^d_\tau p^d_k &= -D^1 H_d(x^d_k, p^d_k, u^d_k), \quad \text{(168)}
    \\
    0 &= D^3 H_d(x^d_k, p^d_k, u^d_k), \quad \text{(169)}
    \\
    p_0 &= D^1 \phi_0(x_0, t_0)^T \lambda_0, \quad p_n = -D^1 \phi_n(x_n, t_n)^T \lambda_n. \quad \text{(170)}
\end{align}
\]

**Lemma 37** The algorithm defined by (167), (168) and (169) is symplectic.

**PROOF.** We omit the proof since it proceeds as before.

### 7.5 Discrete maximum principle v.s. discretization of the Pontryagin maximum principle

So far we have considered two methods for obtaining a symplectic algorithm that integrates the necessary conditions for optimality. The first method, which applies only to a certain class of problems, consists of discretizing the necessary conditions obtained from the Pontryagin maximum principle once the control as been expressed as function of \((x, p)\). The second method consists in using the discrete maximum principle. In this section, we show that under certain assumptions both methods are equivalent, that is we prove the commutative
where \( \bar{H} \) is defined by (151), DMHP stands for discrete modified Hamilton’s principle, PMP stands for Pontryagin maximum principle, and DMP stands for discrete maximum principle.

We recall the required assumptions to prove the equivalence of the diagram. We assume that (149) can be solved for \( u \) as a function of \((x, p)\) and that the initial and final states \( x(t_f) = x_f \) and \( x(t_0) = x_i \) are given. In addition, we impose \( g_d = g \) and \( f_d = f \).

To discretize the Hamiltonian system defined by \( \bar{H} \), we use the discrete modified Hamilton’s principle:

\[
0 = \delta S^\bar{H}_d = \delta \left( \tau \sum_{k=0}^{n-1} \langle p^d_k, \Delta^d x^d_k \rangle - \bar{H}(x^d_k, p^d_k, u^d_k) \right)
\]

(172)

for any variations of \((x^d_k, p^d_k)\) and \( \delta x_0 = \delta x_n = 0 \). One can readily check that (172) can also be written in an equivalent form as:

\[
0 = \delta S^\bar{H}_d = \delta \left( \tau \sum_{k=0}^{n-1} \langle p^d_k, \Delta^d x^d_k \rangle - H_d(x^d_k, p^d_k, u^d_k) \right)
\]

(173)

for any variations of \((x^d_k, p^d_k, u^d_k)\) and \( \delta x_0 = \delta x_n = 0 \) where \( u^d_k \) is now considered as an independent variable. In addition since \( f = f_d \) and \( g = g_d \), \( H = H_d \), and we conclude that the discrete modified Hamilton’s principle as formulated and the discrete maximum principle are equivalent.

### 7.6 The Heisenberg optimal control problem

The Heisenberg problem (Brockett [6], Bloch et al. [3]) refers to under actuated optimal control problems which are controllable. For instance, consider a particle that has two actuators in the \((x, y)\)-plane and with velocity in the
direction defined by \( \dot{z} = y\dot{x} - xy \). This system is controllable, however, to reach a point \((a > 0, 0, 0)\) from the origin \((0, 0, 0)\) requires a non-trivial control vector. In the following, we study the Heisenberg problem to illustrate the approaches we have developed above. This problem formulates as:

\[
\min_{u=(u_1,u_2)} \int_{t_0}^{t_f} \langle u, u \rangle dt ,
\]  

(174)

subject to

\[
\begin{align*}
\dot{x} &= u , \\
\dot{y} &= v , \\
\dot{z} &= uy - vx ,
\end{align*}
\]  

(175) \hspace{1cm} (176) \hspace{1cm} (177)

and to the boundary conditions:

\[
(x(t_0), y(t_0), z(t_0)) = (0, 0, 0) , \quad (x(t_f), y(t_f), z(t_f)) = (a > 0, 0, 0) .
\]

This is a hard constraint problem, therefore the transversality conditions are of no use; They yield \(2n\) equations but introduce \(2n\) new variables.

Define \(H\) as

\[
H(q, p, u) = \frac{1}{2} \langle u, u \rangle + \langle p, \dot{q} \rangle ,
\]

where \(q = (x, y, z)\) and \(p = (p_x, p_y, p_z)\). The Pontryagin maximum principle yields:

\[
\begin{align*}
\dot{q} &= \frac{\partial H}{\partial p}(q, p, u) , \\
\dot{p} &= -\frac{\partial H}{\partial q}(q, p, u) , \\
0 &= \frac{\partial H}{\partial u}(q, p, u) .
\end{align*}
\]  

(178) \hspace{1cm} (179) \hspace{1cm} (180)

Equation (180) allows us to solve for \(u\) as a function of \((q, p)\):

\[
\begin{align*}
u_1 &= p_x + p_z y , \\
u_2 &= p_y - p_z x ,
\end{align*}
\]  

(181)

Hence, equations (178)-(179) become:

\[
\begin{align*}
\dot{q} &= \frac{\partial H}{\partial p}(q, p) , \\
\dot{p} &= -\frac{\partial H}{\partial q}(q, p) ,
\end{align*}
\]

(182) \hspace{1cm} (183)
where

\[ \bar{H}(q, p) = H(q, p, u(q, p)) = -\frac{1}{2}(p_x^2 + p_y^2) - p_x p_z y + p_y p_z x \]

Equations (182) and (183) are of the same form as the Hamilton equations. Therefore, the necessary conditions for optimality yield a Hamiltonian system with Hamiltonian function \( \bar{H} \). We now prove that \( \bar{H} \) is degenerate at the origin, and so is the Legendre transform. The Hessian of \( \bar{H} \) is:

\[
\left( \frac{\partial \bar{H}}{\partial (q, p)} \right) = \begin{pmatrix}
-1 & 0 & -y \\
0 & -1 & x \\
-y & x & 0
\end{pmatrix}
\]

Thus, \( \text{det} \left( \frac{\partial \bar{H}}{\partial (q, p)} \right) = x^2 + y^2 \), i.e., the determinant of the Hessian of \( \bar{H} \) is singular at \((0, 0)\). As a result, it is not, \textit{a priori}, possible to define a Lagrangian function associated with the Hamiltonian \( \bar{H} \) using the Legendre transform. Therefore, the discrete modified Hamilton’s principles (DMHP) must be used to discretize Eqns. (182) and (183). One cannot use a discrete Hamilton’s principles (DHP) for instance because the system is not Lagrangian. This point is of importance. It motivates the need to introduce the variational principles presented in this paper, as previous works on variational principles mostly focused on systems with non-degenerate Lagrangian functions. To discretize the necessary conditions, we choose the geometry associated with the Störmer rule and using DMHP (definition 3) to eventually find the following symplectic algorithm:

\[ \Delta r q_k = D_2 \bar{H}(q_k, p_{k+1}) , \]
\[ \Delta r p_k = -D_1 \bar{H}(q_k, p_{k+1}) . \]

Let us now discretize the Heisenberg problem using the second approach, based on the use of the discrete maximum principle. We first discretize the problem statement:

\[ \min_{u_k=(u_{1,k},u_{2,k})} \frac{1}{2} \sum_{k=0}^{n-1} \langle u_k, u_k \rangle , \]

subject to

\[ \text{(187)} \]

\[ \text{Using Lagrange multipliers one can define a Legendre transform and find a Lagrangian function associated with the system. We refer to Bloch [3] for a presentation of this technique that involves variational principles with constraints.} \]
\[ \Delta \tau x_k = u_{1,k}, \quad (188) \]
\[ \Delta \tau y_k = u_{2,k}, \quad (189) \]
\[ \Delta \tau z_k = u_{1,k}y_k - u_{2,k}x_k. \quad (190) \]

Define the discrete augmented cost function \( J_a \):
\[
J_a = \sum_{k=0}^{n-1} H_d(q_k, p_{k+1}, u_k) - \langle p_{k+1}, \Delta \tau q_k \rangle, \quad (191)
\]
where \( H_d(q_k, p_{k+1}, u_k) = \langle u_k, u_k \rangle + \langle p_{k+1}, q_k \rangle \) and \( q_k = (x_k, y_k, z_k) \). To find discrete necessary conditions for optimality we set the variations of \( J_a \) to zero, and we obtain:
\[
\Delta \tau q_k = D_2 \bar{H}_d(q_k, p_{k+1}, u_k), \quad (192)
\]
\[
\Delta \tau p_k = -D_1 \bar{H}_d(q_k, p_{k+1}, u_k), \quad (193)
\]
\[
0 = D_3 \bar{H}_d(q_k, p_{k+1}, u_k). \quad (194)
\]

Equation (192) allows us to find \( u_k \) as a function of \((q_k, p_{k+1})\):
\[
u_{1,k} = p_{x,k+1} + p_{z,k+1}y_k, \quad u_{2,k} = p_{y,k+1} - p_{z,k+1}x_k. \quad (195)
\]

We then substitute these expressions into equations (192)-(193):
\[
\Delta \tau q_k = D_2 \bar{H}_d(q_k, p_{k+1}) , \quad (196)
\]
\[
\Delta \tau p_k = -D_1 \bar{H}_d(q_k, p_{k+1}) , \quad (197)
\]
where \( \bar{H}_d(q_k, p_{k+1}) = H_d(q_k, p_{k+1}, u_k(q_k, p_{k+1})) \). By virtue of the commutative diagram, (196) and (197) define the same symplectic algorithm as (182) and (183).

In this example, we chose a trivial discretization of the dynamics and of the cost function; \( f = f_d \) and \( g = g_d \). Other algorithms may be obtained using nontrivial discretizations. In that case the equivalence principle may not hold but the algorithm we obtain will still be symplectic. In addition, in this example we did not take into account any boundary conditions since we have seen earlier in the paper that both methods yield comparable transversality conditions. Finally, as in discrete dynamics, the discrete maximum principle may be modified in order to yield symplectic-energy conserving algorithms. We add an independent parameter \( \tau_k \) and consider the time as a generalized coordinate, the optimal control problem then formulates as follows:
\[
\min_u \sum_{k=0}^{n-1} g_d(x^d_k, u^d_k)(t_{k+1} - t_k) = \sum_{k=0}^{n-1} g_d(x^d_k, u^d_k)\Delta \tau t_k \tau. \quad (198)
\]
subject to the dynamics

\[
\Delta_t^d x_k^d = \Delta_t^d t_k^d f_d(x_k^d, u_k^d).
\] (199)

8 Conclusions

In this paper we have presented a general framework that allows one to study discrete systems. We have introduced variational principles on the tangent and cotangent bundles that are the discrete counterpart of the known principles of critical action for Lagrangian and Hamiltonian dynamical systems. We have shown that they allowed us to recover most of the classical symplectic algorithms. In the future, we will try to derive additional symplectic algorithms such as the symplectic partitioned Runge-Kutta algorithm. In addition, we have seen that by increasing the dimensionality of the configuration space, symplectic algorithms may be transformed into symplectic-energy conserving algorithms. When time is a generalized coordinate, the dynamical system is subject to an energy constraint and we are able to adapt our variational principles to take into account such a constraint. In the same manner, our approach may be modified to derive symplectic algorithms to integrate non-autonomous dynamical and control systems with (non-holonomic) constraints. We have also identified a class of coordinate transformations that leaves the variational principles presented in this paper invariant and developed a discrete Hamilton-Jacobi theory. This theory allows us to relate the energy error in the integration using different set of coordinates. Finally, for optimal control problems we have developed a discrete maximum principle that yields discrete necessary conditions for optimality. These conditions are in agreement with the usual conditions obtained from Pontryagin maximum principle. In future research, we want to use the general framework introduced in this paper to develop variational principles for multi-symplectic algorithms, that is a spacetime discretization will be used instead of the time discretization. Such a formulation would allows us to develop efficient numerical algorithms for simulation of the motion of rigid bodies and complex interconnected systems.

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