UNIVERSIDAD COMPLUTENSE DE MADRID
FACULTAD DE CIENCIAS MATEMÁTICAS

TESIS DOCTORAL

Discrete Mechanics for Forced and Constrained Systems

Mecánica Discreta para Sistemas Forzados y Ligados

MEMORIA PARA OPTAR AL GRADO DE DOCTOR

PRESENTADA POR

Rodrigo T. Sato Martín de Almagro

DIRECTOR

David Martín de Diego

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DECLARACIÓN DE AUTORÍA Y ORIGINALIDAD DE LA TESIS PRESENTADA PARA OBTENER EL TÍTULO DE DOCTOR

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Doctoral Thesis

Discrete Mechanics for Forced and Constrained Systems

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Advisor:
Martín de Diego, David

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Abstract

Geometric mechanics is a branch of mathematics that studies classical mechanics of particles and fields from the point of view of geometry and its relation to symmetry. One of its most interesting developments was bringing together numerical analysis and geometry by relating what is known as discrete mechanics with numerical integration. This is called geometric integration. In the last 30 years this latter field has exploded with research from the purely theoretical to the strictly applied.

Variational integrators are a type of geometric integrators arising naturally from the discretization process of variational principles in mechanics. They display some of the most salient features of the theory, such as symplecticity, preservation of momenta and quasi-preservation of energy. These methods also apply very naturally to optimal control problems, also based on variational principles. Unfortunately, not all mechanical systems of interest admit a variational formulation. Such is the case of forced and nonholonomic mechanical systems.

In this thesis we study both of these types of systems and obtain several new results. By geometrizing a new technique of duplication of variables and applying it, we were able to definitely prove the order of integrators for forced systems by using only variational techniques. Furthermore, we could also extend these results to the reduced setting in Lie groups, leading us to a very interesting geometric structure, Poisson groupoids. In addition, we developed new methods to geometrically integrate nonholonomic systems to arbitrary order preserving their constraints exactly. These methods can be seen as nonholonomic extensions of variational methods, and we were able to prove their order, although not through variational means. These methods have a nice geometric interpretation and thanks to their closeness to variational methods, they can be easily generalized to other geometric settings, such as Lie group integration. Finally, we were able to apply these new methods to optimal control problems.

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of yet, but I hope they will in the near future. I should also thank Alexander Schmeding, who was really helpful during my stay in Trondheim in trying to understand Michor's papers, Sina Ober-Blöbaum, for having David and me for a week in Oxford with you and Fernando, and also Sigrid Leyendecker, for her interest in my research and the new opportunity she has given me in Erlangen. Por otro lado, debo también mencionar a dos profesores de la facultad de ciencias físicas de la UCM, a David Gómez-Ullate, quien fue mi primer mentor en el mundo de la investigación, y a Luis J. Garay, quien me animó a contactar con David Martín tras constatar mi interés por la mecánica geométrica.

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Contents

Resumen

La **mecánica clásica** es un campo tan fundamental para la física como la **geometría** lo es para las matemáticas. Ambos están interrelacionados y su estudio conjunto así como sus interacciones forman lo que hoy se conoce como la **mecánica geométrica** [vease, por ejemplo, AM78; Arn89; Hol11a; Hol11b].

Hoy es bien sabido que el concepto de simetría tiene importantes consecuencias para los sistemas mecánicos. En particular, la evolución de los sistemas mecánicos suele mostrar ciertas propiedades de preservación en forma de cantidades conservadas del movimiento o preservación de estructuras geométricas. Ser capaces de capturar estas propiedades es vital para tener una imagen fiel, tanto en términos cuantitativos como cualitativos, de cara al estudio de estos sistemas. Esto tiene gran importancia en el campo teórico y también el aplicado, como en la ingeniería.

La experimentación en laboratorios y la generación de prototipos son procesos costosos y que requieren de tiempo, y para determinados sistemas pueden no ser siquiera factibles. Con la llegada el ordenador, simular y experimentar con sistemas mecánicos de forma rápida y económica se convirtió en una realidad. Desde sencillas simulaciones balísticas para alumnos de secundaria a simulaciones de dinámica molecular a gran escala; desde la planificación de trayectorias para vehículos autónomos a la estimación de movimientos en robots bípedos; desde costosas simulaciones basadas en modelos físicos para la industria de la animación a la simulación de sólidos rígidos y deformables en tiempo real para la industria del videojuego, el tratamiento numérico de sistemas de complejidad creciente se ha convertido en una necesidad. Naturalmente surgieron nuevos algoritmos capaces de conservar gran parte de las propiedades geométricas de estos sistemas, configurando lo que ahora se conoce como **integración geométrica** [vease SC94; HLW10].

En los últimos 20 a 30 años se han dado grandes pasos en esta dirección, con el desarrollo de métodos que conservan energía, métodos simplécticos y multisimplécticos, métodos que preservan el espacio de configuración y más. Aún así, la investigación en esta área está todavía lejos de acabar. Por ejemplo, los sistemas sometidos a fuerzas externas y con ligaduras ofrecen ciertas dificultades que han de ser abordadas, y esta tesis se dedica a explorar estos dos casos ofreciendo nuevos desarrollos y resultados.

La mecánica discreta puede verse como una versión a paso finito de la *mecánica continua*. Ello significa que en vez de tratar trayectorias continuas que podemos determinar en cualquier instante a lo largo de la evolución del sistema, únicamente tenemos una serie de imágenes estáticas o fotogramas en un conjunto fijo de instantes. La **mecánica discreta** nos ofrece un punto de vista muy interesante de cara a la integración geométrica [véase MW01].

Los sistemas mecánicos continuos libres son gobernados por un **principio variacional** llamado *principio de Hamilton*. Este principio indica que la naturaleza favorece que la trayectoria de un sistema mecánico sea tal que extremice el valor de un cierto funcional. Esto nos permite obtener las ecuaciones del movimiento de un sistema de una forma

sistemática. Lo mismo ocurre en el caso de la mecánica discreta, gobernada por la versión discreta del principio de Hamilton.

Los **integradores variacionales** son métodos numéricos geométricos obtenidos mediante la aproximación de este principio variacional y se aplican para obtener ecuaciones del movimiento aproximadas. Esto contrasta con el uso común de los métodos numéricos tradicionales en los que se parte directamente de las ecuaciones del movimiento y se toma una aproximación de ellas. Los integradores variacionales son siempre simplécticos y tienen excelentes propiedades tanto estadísticas como cualitativas, mostrando un muy buen comportamiento de la energía en grandes escalas temporales.

Los sistemas mecánicos forzados y algunos sistemas con ligaduras llamadas **no-holónomas** [BM02; Blo15] son *a priori* no variacionales, pero sus ecuaciones del movimiento son marcadamente similares a las de los sistemas variacionales. Tratar de generar métodos numéricos para este tipos de sistemas de forma análoga a como se procede con los integradores variacionales parece sensato. En su tesis [MW01], Matthew West mostraba como extender los integradores variacionales a los sistemas forzados, pero algunos problemas quedaron sin resolver de forma totalmente satisfactoria. En particular, el trabajo posterior de Patrick and Cuell parece invalidar algunos de los resultados de esta tesis. También se tratan los sistemas ligados holónomos, pero deja a un lado el caso no-holónomo.

Quizás una de las propiedades más deseables que ha de satisfacer un método numérico para un sistema ligado es precisamente el respetar las propias ligaduras. Los sistemas no-holónomos son un tipo particular de sistema mecánico ligado, capaces de mostrar comportamientos desconcertantes y extraños vistos desde el prisma de los sistemas libres. Ejemplos prototípicos de sistemas no-holónomos son tales como ruedas y bolas que ruedan sin deslizamiento o cuchillas y patines que se deslizan. Estos tienen importantes aplicaciones en automática y robótica.

El objetivo principal de esta tesis ha sido tratar de entender mejor estos sistemas y estudiar cómo tratar estos casos numéricamente en el contexto de los integradores variacionales. Dado que los sistemas ligados pueden entenderse como casos particulares de sistemas forzados, nuestro estudio comenzó con los métodos para sistemas forzados con la esperanza de resolver algunos de sus problemas pendientes y siempre teniendo en mente su posible aplicación al caso no-holónomo.

Esto nos llevó a estudiar de los sistemas forzados desde un nuevo prisma, como sistemas variacionales en dimensiones superiores. En particular, utilizando los resultados de un reciente trabajo de Chad Galley [Gal13]. La teoría de Galley permite interpretar un sistema mecánico forzado como un sistema con variables duplicadas. La teoría muestra ciertas propiedades que apuntan hacia una cierta estructura geométrica subyacente: los **grupoides de Lie**. Nosotros estudiamos una versión geometrizada de la teoría y arrojamos luz sobre sus propiedades. Finalmente utilizamos esta teoría para resolver uno de los problemas no resueltos de los integradores forzados: el correcto análisis del error. Estos resultados también han sido extendidos y aplicados al caso de sistemas reducidos por simetrías, en particular, los definidos sobre grupos de Lie.

Dada la naturaleza bastante compleja de las fuerzas de no-holónomas y su relación con las ligaduras en el caso discreto, no hemos sido capaces de aplicar estos resultados anteriores al problema que originalmente queríamos tratar. Aún así, hemos sido capaces de desarrollar un nuevo método de integración geométrica para sistemas no-holónomos que preservan las ligaduras de forma exacta y que tienen una estructura similar a la de un integrador variacional. Algunos de los métodos pre-existentes era métodos de baja precisión [CM01; FIM08; LMS04]. Otros métodos existentes de orden alto no eran

integradores adaptados a la estructura especial de los sistemas mecánicos [HLR89; Jay93; Jay03], y el único que sí estaba adaptado dependía de ciertos parámetros muy particulares [Jay09]. Nosotros somos capaces de ofrecer toda una familia de métodos de precisión arbitrariamente alta, la cuál hemos podido demostrar, y que además pueden entenderse como una extensión de los métodos de [CM01; LMS04]. Además hemos sido capaces de extender nuestros métodos para ser aplicados tanto en los casos en grupos de Lie como en los de **control óptimo**.

La estructura de la tesis es la siguiente:

- En el **capítulo 2** presentamos las herramientas necesarias para desarrollar los resultados de este trabajo. Éste está dividido en tres partes principales:
  - Geometría diferencial general de variedades y fibrados, con énfasis particular en el fibrado tangente y cotangente y en los grupos y grupoides de Lie.
  - Cálculo de variaciones, principalmente resultados clásicos con una breve sección sobre control óptimo.
  - Teoría básica de la integración numérica, con varios resultados importantes y extensión a grupos de Lie.

  El lector avezado en la materia puede omitir este capítulo. Los capítulos posteriores lo referenciarán cuando sea necesario.

- El capítulo 3 es una introducción a la mecánica geométrica. Tiene secciones específicas sobre mecánica discreta, con especial interés en los integradores variacionales, tanto en espacios vectoriales como para grupos de Lie. Casi todos los resultados de este capítulo son conocidos, aunque hacia el final (a partir de la sección 3.4.4), cuando analizamos métodos en grupos de Lie presentamos una derivación completa de métodos variacionales de order alto. También presentamos la tangente segunda trivializada de una retracción, su interpretación geométrica y algunas de sus propiedades.

- El capítulo 4 está dedicado a los sistemas forzados, comenzando con el principio de Lagrange-D'Alembert en el caso continuo. También comentamos los problemas que hay para probar el orden de los métodos de integración forzados obtenidos en [MW01]. Ello sirve de motivación para tratar de analizar los sistemas forzados de una forma distinta. Posteriormente pasamos a presentar el trabajo de Galley [Gal13], y procedemos a su análisis geométrico. Tras aplicar esta teoría para probar el orden de los integradores forzados, pasamos al caso de los sistemas forzados en grupos de Lie. Allí, la geometría que aparece tras el proceso de reducción es la de los grupoides de Poisson. Algunos de los resultados de este capítulos han sido objeto de una reciente publicación [MS18b], y otro preprint [MS19] incluyendo los restantes.

- El capítulo 5 versa sobre los sistemas con ligaduras. Comenzamos con un estudio sobre los sistemas continuos holónomos y no-holónomos, resaltando sus semejanzas y sus diferencias. En particular, los sistemas no-holónomos son no variacionales y su teoría discreta es bastante deficiente y sin resultados que puedan ayudarnos de cara a la integración numérica. Dado que los sistemas no-holónomos presentan una estructura natural de sistema de ecuaciones algebro-diferenciales particionado de índice 2 (consúltese la sección 2.3.5), proponemos un nuevo método numérico

para este tipo de sistemas. Pasamos a realizar el análisis numérico necesario para demostrar que el orden del método propuesto es el correcto y luego lo particularizamos al caso de la mecánica no-holónoma. Como la teoría subyacente se basa en los integradores variacionales, somos capaces de pasar al contexto de los grupos de Lie de forma fácil y manteniendo las mismas estimaciones de error. Ofrecemos, además, varios experimentos numéricos para ilustrar el método. Para terminar, mostramos cómo aplicar estos métodos a problemas de control óptimo. La mayoría de estos resultados están disponibles en preprints [Sat18; MS18a] y han sido presentados para su publicación.

- El capítulo 6 resume los resultados de la tesis y propone una serie de cuestiones y problemas todavía no resueltos que pueden ser objeto de trabajos futuros.

Chapter 1

Introduction

Classical mechanics is as fundamental to Physics as *geometry* is to Mathematics. Both fields are interconnected and the joint study of these and their interactions make up what is known today as **geometric mechanics** [see, for instance, AM78; Arn89; Hol11a; Hol11b].

Nowadays it is well-known that the concept of symmetry has important consequences for mechanical systems. In particular, the evolution of mechanical systems tends to display certain conservation properties in the form of conserved quantities or conserved geometric structures. Capturing these properties are very important for the overall faithful quantitative and qualitative study of the system, and it has important consequences both in the theoretical and applied sciences fields, such as engineering.

Real-life experimentation in laboratories and prototyping are costly and time consuming endeavors, and for certain systems they may not even be feasible. With the advent of the digital computer, the possibility to simulate and experiment with mechanical systems in a fast and cost-effective way was possible. From small ballistic simulations for high-school students to large-scale molecular dynamics; from trajectory planning of autonomous vehicles, to motion estimation for bipedal robots; from off-line physically-based simulations for the animation industry to real-time efficient rigid and deformable bodies simulation for video games, the numerical treatment of increasingly complex systems is a necessity. Naturally, new algorithms capable of preserving a big part of the geometric properties of these systems began to appear, configuring what we now know as **geometric integration** [see SC94; HLW10].

In the last 20 to 30 years huge strides have been made in this direction, with the development of energy-preserving methods, symplectic and multisymplectic integration, methods preserving the structure of the configuration space and more. Still, research in this area is far from over. For instance, mechanical systems subject to **external forces** or **constraints** offer some difficulties that must be addressed, and this thesis is dedicated to explore these two cases offering new developments and results.

Discrete mechanics can be thought of as a finite time-step version of *continuous mechanics*. This means that instead of having a continuous trajectory which we can determine at any given instant along the evolution of the system, we only have a series of discrete frames or still images at a certain set of instants. **Discrete mechanics** provides us with a very interesting point of view for geometric integration [see MW01].

Free continuous mechanical systems are governed by a **variational principle** known as *Hamilton's principle*. This principle points out that nature favors that the trajectory of a mecanical system be such that it extremizes a certain functional. This allows us to

obtain the equations of motion for a system in a systematic way. The same happens in the case of discrete mechanics, governed by the discrete version of Hamilton's principle.

Variational integrators are geometric numerical methods obtained by approximating this variational principle and using it to obtain approximate equations of motion. This is in contrast with the application of usual numerical methods which starts from the equations of motion, approximating them instead of something more fundamental. Variational integrators are always symplectic, thus offering good statistical and qualitative properties, and they display very good long term energy behavior.

Forced mechanical systems and some constrained systems called **nonholonomic** [BM02; Blo15] are *a priori* non-variational, but their equations of motion are very similar to their variational counterparts. Generating numerical methods for these systems in analogy with variational integrators seems like a sensible choice. In his thesis Matthew West [MW01] shows how to extend these variational integrators to forced systems, but some issues were not resolved satisfactorily. Particularly, the later work of Patrick and Cuell [PC09] seems to invalidate some of the results of this thesis. West also treats some constrained systems, but leaves the nonholonomic case untreated.

For constrained systems, perhaps one of the most desirable features of a numerical method is precisely the preservation of the constraint while disturbing all other properties as little as possible. Nonholonomic mechanical systems are a particular type of constrained system capable of displaying bizarre and puzzling behavior from the viewpoint of free systems. Prototypical examples of nonholonomic mechanical systems are wheels and balls rolling without slipping or sliding knife edges and skates. These systems find important application in robotics and automation.

The main goal of this thesis was to better understand these systems and study how to treat them numerically in the context of variational integrators. As constrained systems can be seen as particular kinds of forced systems, we began studying forced integrators with the hopes to solve some of their remaining issues and with our minds set on its application to the nonholonomic case.

This lead us to study a new way of understanding forced systems as variational systems in higher dimension, particularly via the recent work of Chad Galley [Gal13]. Galley's theory allows us to see any forced mechanical system as a free and variational mechanical system with duplicated variables. The theory displays certain properties that point nicely to a geometric structure behind it: **Lie groupoids**. We study this geometrized version of the theory and shed light on its properties and we finally apply this to tackle one of the unresolved issues left with forced integrators: correct error analysis. These results have also been extended and applied to symmetry-reduced systems, particularly on Lie groups.

Due to the complex nature of the nonholonomic forces and their relation with the constraints in the discrete setting, we were not able to apply the former results to the original case we intended. Nevertheless, we were able to generate a new geometric method for nonholonomic systems which preserves the constraints exactly and has a structure similar to a variational method. Some of the existing methods were bound to low order accuracy [CM01; FIM08; LMS04]. Some preexisting high-order methods were not designed for mechanical systems [HLR89; Jay93; Jay03], and some that were [Jay09] depended on some very particular parameters. We were able to offer an entire family of arbitrarily high-order which we were able to prove and can be seen as an extension of the methods of [CM01; LMS04]. We also extended our method to the case of Lie groups and apply them for **optimal control** problems.

The structure of this thesis is as follows:

- **Chapter 2** presents all the mathematical tools necessary to develop the results of this work. It is divided in three main parts:
  - General differential geometry of manifolds and fibre bundles, with particular emphasis on the tangent and cotangent bundles and Lie groups and groupoids.
  - Calculus of variations, mostly classic results, with a small section on optimal control.
  - Basic theory of numerical integration, with some important results and extensions to Lie groups.

  The reader comfortable with those topics may skip this chapter. Later chapters will reference it when necessary.

- Chapter 3 is an introduction to geometric mechanics. It has specific sections on discrete mechanics, with special interest on variational integrators on both vector spaces and Lie groups. Most results here are well-known but towards the end (beginning from section 3.4.4), when we study Lie group methods we present a complete derivation of high-order variational integrators. We also present the second trivialized tangent of a retraction, its geometric interpretation as well as some of its properties.

- Chapter 4 is dedicated to forced systems, starting from the Lagrange-D'Alembert principle in the continuous case. We comment on the problem of proving the accuracy of forced integrators obtained as in [MW01]. This serves as a motivation to try and analyze forced systems in a different way. Then we proceed to introduce the work of Galley [Gal13], and begin with its geometric analysis. After applying this theory to finally prove the accuracy of forced integrators, we move on to the Lie group setting. There the geometry that appears after reduction is that of Poisson groupoids. Some of the results of this chapter have been the object of a recent publication [MS18b], and another preprint compiling the rest [MS19].

- Chapter 5 discusses constrained systems. We begin with a study of continuous holonomic and nonholonomic systems, highlighting their similarities and differences. In particular nonholonomic systems are non-variational and their discrete theory is lacking, with no helpful results for numerical integration. As nonholonomic systems naturally present the structure of partitioned index 2 differential-algebraic systems of equations (DAEs) (refer to 2.3.5), we propose a new numerical method for these. We proceed with the numerical analysis necessary to show that the proposed method is of the right order and then we particularize to the case of nonholonomic mechanics. As the underlying theory is based around variational integrators, we can easily move to the Lie group setting maintaining the same error estimates. We also offer a plethora of numerical tests. Finally, we show how to apply these methods to optimal control problems. Most of the results of this chapter are available as preprints [Sat18; MS18a] and have been submitted for publication.

- Chapter 6 summarizes the results of this thesis and poses some open problems not addressed in this thesis that may be subject of future work.

Chapter 2

Mathematical tools

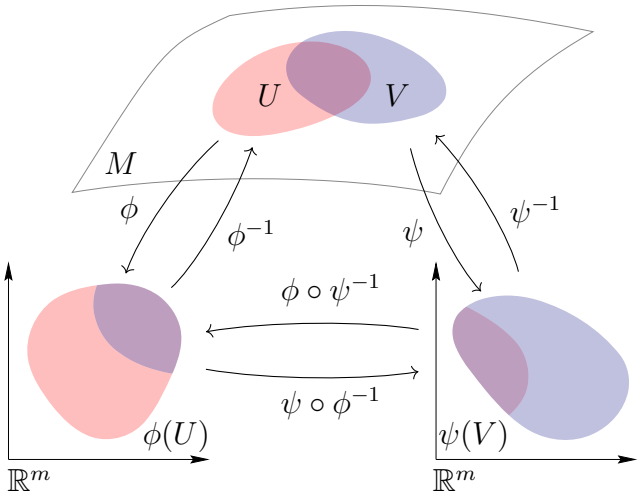
2.1 Differential geometry

A big part of this section is based on the books [Lee03; Fec06]. Further references can be found throughout the text for notions not found in those books or not taken from them.

2.1.1 Smooth manifolds

A **smooth manifold** $(M, \mathcal{A})$ of dimension $m \in \mathbb{N}$ is a topological manifold M of the same dimension together with a smooth structure given by a maximal smooth atlas, $\mathcal{A}$. For the purpose of this work we will assume that the manifolds we work with have an obvious smooth structure and we will thus refer to the smooth manifold simply as M.

Every chart $(U, \phi) \in \mathcal{A}$, with $U \subset M$, $\phi : U \to \widehat{U} \subseteq \mathbb{R}^m$, is consequently smooth. This means that the map ϕ is a diffeomorphism, i.e. smooth and bijective with smooth inverse. Here smooth will be taken as equivalent to C^∞. Clearly, for any two charts $(U, \phi), (V, \psi) \in \mathcal{A}$ such that $U \cap V \neq \emptyset$, the transition map $\psi \circ \phi^{-1} : \phi(U \cap V) \to \psi(U \cap V)$, must also be a diffeomorphism.



If we work locally on a smooth manifold, we may choose a chart (U, ϕ) such that it covers the region of interest. This way we can make use of the local identification with $\widehat{U} \subset \mathbb{R}^m$ and represent a given point $x \in U$ with the (local) coordinates induced by the chart, that is, $\phi(x) = (x^1, ..., x^m)$. To simplify the notation, one usually omits ϕ and

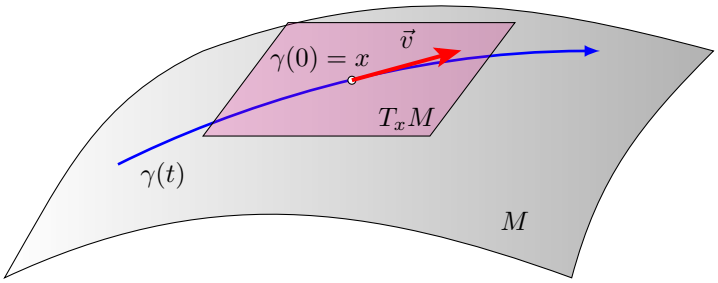
directly identify x with the coordinates, although that must always be thought of as an abuse of notation.

The tangent and cotangent spaces of a manifold

A **smooth curve** γ on M that passes through $x \in M$ is a smooth map $\gamma : I \subseteq \mathbb{R} \to M$, such that $\gamma(t_0) = x$ for some $t_0 \in I$. Without loss of generality we may assume that $t_0 = 0$. Given two curves γ_1 and γ_2 passing through x, we say that they are tangent at x if there exists a chart (U, ϕ) with $x \in U$, such that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\phi \circ \gamma_1)(t)\bigg|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t}(\phi \circ \gamma_2)(t)\bigg|_{t=0}$$

This generates an equivalence class $[\gamma]$, which is the tangent vector of γ at x. The set of all these equivalence classes at x conforms the **tangent space** of M at x, denoted by T_xM.



Let us define $T_x\phi : T_xM \to T_{\phi(x)}\widehat{U} \cong \mathbb{R}^m$ as the map that sends equivalence classes to vectors, i.e., $T_x\phi\,([\gamma]) = \frac{\mathrm{d}}{\mathrm{d}t}(\phi \circ \gamma)(t)\big|_{t=0} = \vec{v}$. This is in fact a bijection. If we define a vector space structure on T_xM from the one on $\mathbb{R}^m$ such that $T_x\phi$ acts linearly, that is,

$$\begin{aligned} v + w &= (T_x\phi)^{-1}\,(\vec{v} + \vec{w}) \quad \text{with } v, w \in T_xM, \vec{v}, \vec{w} \in \mathbb{R}^n, \\ av &= (T_x\phi)^{-1}\,(a\vec{v}) \qquad\qquad\qquad\qquad \text{with } a \in \mathbb{R}, \end{aligned}$$

then one can prove that this structure is independent of the choice of chart, and thus T_xM is indeed a vector space of dimension n.

Given any chart (U, ϕ), using the canonical basis of $\mathbb{R}^m$, $(e_1, ..., e_m)$ we can obtain a basis on T_xM by using the construction

$$\gamma^i(t) = \phi^{-1}\left(\phi(x) + te_i\right), \quad \text{with } i = 1, ..., m.$$

The resulting basis, $((\partial/\partial x^1)_x, ..., (\partial/\partial x^m)_x)$, where $(\partial/\partial x^i)_x = \frac{\mathrm{d}\gamma^i}{\mathrm{d}t}(0)$, is called the *natural basis of that chart*. We will sometimes abbreviate this as $((\partial_{x^1})_x, ..., (\partial_{x^m})_x)$ or even $(\partial_{x^1}, ..., \partial_{x^m})$.

Another important space at a point x is the **cotangent space**, denoted by T_x^*M, which is defined as the dual space of T_xM, i.e. $T_x^*M = (T_xM)^*$. The elements of a cotangent space are called covectors, and as elements of a dual space they are linear forms, that is, if $\alpha \in T_x^*M$, then $\alpha : T_xM \to \mathbb{R}$. The dual basis associated with the natural basis on T_xM, is $((\mathrm{d}x^1)_x, ..., (\mathrm{d}x^m)_x)$ or simply $(\mathrm{d}x^1, ..., \mathrm{d}x^m)$. We will sometimes denote the natural pairing of vectors and covectors as $\langle \cdot, \cdot \rangle : T_x^*M \times T_xM \to \mathbb{R}$, $(\alpha, v) \mapsto \langle \alpha, v \rangle$.

A generalization of these objects are **tensors**. A tensor K of type $\binom{p}{q}$ at $x \in M$ is a multilinear map

$$K : \underbrace{T_xM \times \cdots \times T_xM}_{q} \times \underbrace{T_x^*M \times \cdots \times T_x^*M}_{p} \to \mathbb{R}.$$

Under such a definition a vector can be seen as a $\binom{1}{0}$-tensor and a covector as a $\binom{0}{1}$-tensor. The space of all $\binom{p}{q}$-tensors a x will be denoted as $\mathcal{T}_q^p(M_x)$, and the space

$$\mathcal{T}(M_x) = \bigoplus_{p,q=0}^{\infty} \mathcal{T}_q^p(M_x),$$

where $\mathcal{T}_0^0(M_x) = M_x$ by convention, is called tensor space. The tensor product operation,

$$\otimes : \mathcal{T}_q^p(M_x) \times \mathcal{T}_{q'}^{p'}(M_x) \to \mathcal{T}_{q+q'}^{p+p'}(M_x),$$

allows us to generate new tensors from others. This can be extended to $\mathcal{T}(M_x)$ which makes $(\mathcal{T}(M_x), \otimes)$ an algebra, the tensor algebra at x.

An important subspace space of $\mathcal{T}_q^p(M_x)$ is the space of alternating (or antisymmetric) $\binom{0}{q}$-tensors, denoted as $\bigwedge^q(T_x^*M)$, whose elements are called q-forms. If $\omega \in \bigwedge^q(T_x^*M)$, then

$$\omega(v_1, ..., v_i, ..., v_j, ..., v_q) = -\omega(v_1, ..., v_j, ..., v_j, ..., v_q), \quad \text{for } \{v_k\}_{k=1}^q \subset T_xM.$$

In this space a new product that generates new forms from other forms can also be defined. First let us define the projection, $\mathrm{Alt} : \mathcal{T}_q^0(M_x) \to \bigwedge^q(T_x^*M)$, as

$$\mathrm{Alt}\,\omega(v_1, ..., v_q) = \frac{1}{q!} \sum_{\sigma \in S_q} (\operatorname{sgn}\sigma)\, \omega(v_{\sigma(1)}, ..., v_{\sigma(q)}).$$

Using this projection we can define the **exterior product** (or *wedge product*) of two forms, $\wedge : \bigwedge^q(T_x^*M) \times \bigwedge^p(T_x^*M) \to \bigwedge^{q+p}(T_x^*M)$, from the tensor product as

$$\omega \wedge \eta = \frac{(q+p)!}{q!p!}\,\mathrm{Alt}\,(\omega \otimes \eta)\,.$$

If we define the space of all forms at x as

$$\bigwedge(T_x^*M) = \bigoplus_{q=0}^{\infty} \bigwedge^q(T_x^*M),$$

then $(\bigwedge(T_x^*M), \wedge)$ is called the exterior algebra.

Another operation commonly defined on forms is the **interior product** with a vector $w \in T_xM$, $\imath_v : \bigwedge^q(T_x^*M) \to \bigwedge^{q-1}(T_x^*M)$, which is just evaluation in the first slot, so that

$$(\imath_w\alpha)\,(v_1, ..., v_{q-1}) = \alpha(w, v_1, ..., v_{q-1}).$$

This means that if α is a 1-form,

$$\alpha(w) = w(\alpha) = \langle \alpha, w \rangle = \imath_w\alpha.$$

Note that by the antisymmetry of forms we have that for any q-form ω with $q \geq 2$, and any pair of vectors u and v,

$$\imath_u\imath_v\omega = -\imath_v\imath_u\omega,$$

which implies that $\imath_u\imath_u = 0$.

Maps between manifolds

Let M, N be two smooth manifolds, not necessarily of the same dimension. We say that the map $F : M \to N$ is smooth if for every $x \in M$ there exist smooth charts (U, ϕ) and (V, ψ), where $x \in U$ and $F(x) \in V$, with $F(U) \subset V$ such that the map $\bar{F} = \psi \circ F \circ \phi^{-1} : \phi(U) \to \psi(V)$ is smooth.

From F we can define a linear map, $T_xF : T_xM \to T_{F(x)}N$, by $T_xF([\gamma]) = [F \circ \gamma]$, called the differential of F at x. If $\dim N = n$, and ψ induces local coordinates $(y^1, ..., y^n)$, then

$$T_xF\left((\partial_{x^i})_x\right) = \frac{\partial F^j(x)}{\partial x^i}(\partial_{y^j})_{F(x)},$$

where $(\partial F^j(x)/\partial x^i)$ is the well-known Jacobian matrix and Einstein's "*summation over repeated indices*" convention has been used and will be used from now on.

We say that T_xF is of rank r if the rank of the Jacobian matrix is r, and we say that $\operatorname{rank} F = r$ at x. If $\operatorname{rank} F$ remains constant for all points in M, then we say that it is of *constant rank*.

We say that $F : M \to N$ is a (smooth) submersion if its differential is surjective everywhere ($\operatorname{rank} F = \dim N$). A particular case of smooth submersions that we will encounter is called projection, which are also surjective and usually denoted by π or pr. Let $\pi : M \to N$ be a surjective submersion, then any smooth map $\sigma : N \to M$ such that $\pi \circ \sigma = \mathrm{Id}_N$ is called a smooth section of π.

We say that $F : M \to N$ is a (smooth) immersion if its differential is injective everywhere ($\operatorname{rank} F = \dim M$). If F is an immersion and injective, then $M \subseteq N$ is said to be an (immersed) submanifold of N, and F is said to be an inclusion map. Inclusions are usually denoted by i and with a hook instead of an arrow, i.e., $i : M \hookrightarrow N$.

The constant rank theorem states that if a smooth map $F : M \to N$ is of constant rank, then:

- if F is surjective, then it is a smooth submersion;
- if F is injective, then it is a smooth immersion;
- if F is bijective, then it is a diffeomorphism.

In the last case, F^{-1} exists everywhere and is smooth, and necessarily $\dim M = \dim N = \operatorname{rank} F$. In that case M and N are said to be diffeomorphic, and we will write $M \cong N$. If this only holds for a neighborhood U, so that $F|_U : U \to F(U)$ is a diffeomorphism, then F is said to be a local diffeomorphism. The inverse function theorem states that if T_pF is invertible at a point x, then there exist connected neighborhoods U_0 of x and V_0 of $F(x)$ such that $F|_{U_0} : U_0 \to V_0$ is a diffeomorphism.

Fields on a manifold

The (smooth) assignment of a tangent vector to each point of $U \subseteq M$ is called a (smooth) **vector field**, denoted by $V(x) \in T_xM$. The set of all vector fields in U is commonly denoted as $\mathfrak{X}(U)$.

A vector field V can thought of as an operator acting on any smooth function, giving a new function, that is, $V : C^\infty(M, \mathbb{R}) \to C^\infty(M, \mathbb{R})$, $f \mapsto Vf$. This action satisfies the properties of a derivation:

- linearity: $V(f + cg) = Vf + c(Vg), \forall f, g \in C^\infty(M, \mathbb{R}), c \in \mathbb{R}$;

- product rule: $V(fg) = (Vf)g + f(Vg)$.

This coincides with the traditional notion of directional derivative.

If we had two vector fields, V and W, we could apply one after the other, that is, WVf or VWf to obtain new functions. Still, neither WV nor VW could be interpreted as a new vector field acting on f because neither acts as a derivation (they do not satisfy the product rule). However, $[V, W] = VW - WV$ can be shown to be a new vector field, that is, it satisfies

$$[V, W](fg) = ([V, W] f) g + f([V, W] g).$$

This is called the **Lie bracket** of the two vector fields.

An **integral curve** of a vector field $V \in \mathfrak{X}(M)$ is a curve fulfilling the condition that its velocity vector at each point coincides with the value of the vector field at said point, that is,

$$\dot{\gamma}(t) = V(\gamma(t)).$$

A vector field can then be interpreted as to be dividing M into a system of integral curves, generating a map

$$\Phi : I \times M \to M,$$

which for a certain $t \in I \subseteq \mathbb{R}$ displaces a point x to $\Phi(t, x) \equiv \Phi_t(x)$. This is called a **(local) flow** or **one-parameter group** of transformations, as it can be interpreted as the group $\mathbb{R}$ acting on the manifold M. It satisfies that $\Phi_t \circ \Phi_s = \Phi_{t+s}$. Note that $\frac{\partial \Phi_t}{\partial t} = (V\Phi)_t$

A smooth distribution $\mathcal{D}$ on M is a smooth assignment to each point $x \in M$ of the subspace spanned by the values at x of a set of smooth vector fields [see Blo15]. Thus $\mathcal{D}_x \subset T_x M$.

A distribution is said to be *involutive* if for any pair of vector fields V, W in $\mathcal{D}$, their Lie bracket $[V, W]$ is also in $\mathcal{D}$. A distribution is said to be *integrable* if through each point $x \in M$ a local submanifold $N \subset M$ can be spanned such that for each point $y \in N$ its tangent spaces equal $\mathcal{D}_y|_N$. If a distribution is integrable, then a maximal extension of a submanifold, a *maximal integral manifold*, passes through each point in M, generating a *foliation*. Frobenius's theorem guarantees that $\mathcal{D}$ is integrable if and only if it is involutive.

In this sense, every vector field in M can be regarded as a 1-dimensional integrable distribution and its integral curves define maximal integral manifolds.

Consider now a smooth map $F : M \to N$ as in the previous section. If V is a vector field on M and F is injective, then F induces a new vector field on its image, $(T_x F)V(x) \in T_{F(x)} N$. This is called a **vector field along** F. Furthermore, if F is a diffeomorphism, then one can define a vector field on all N

$$W(x) = \left(T_{F^{-1}(x)} F\right) \left(V\left(F^{-1}(x)\right)\right).$$

This new vector field can be noted as $F_* V \in \mathfrak{X}(N)$, and is called the **pushforward** of V. We may still abuse this notation, using it when F is only injective as $(T_x F)V(x) = (F_* V)(F(x))$.

In the case where F is surjective, then a vector field on N derived from a vector field on M is only well-defined when for $x \in N$ and $x \in F^{-1}(x)$, $(T_x F)V(x)$ is independent of the choice of x. Such vector fields on M are said to be **projectable**.

As with functions, a vector field V can act on another vector field W to give us a sense of the *rate of change* of W along the flow of V, Φ_t,

$$\mathcal{L}_V W(x) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[T_{\Phi_{\Delta t}(x)} \Phi_{-\Delta t} W(\Phi_{\Delta t}(x)) - W(x)\right].$$

This is what we call the **Lie derivative** of W with respect to V, and it can be shown that

$$\mathcal{L}_V W = [V, W] \, .$$

If f is a smooth function on M, then we define its Lie derivative as

$$\mathcal{L}_V f(x) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[f(\Phi_{\Delta t}(x)) - f(x) \right] .$$

Clearly, with this definition we have that $\mathcal{L}_V f = Vf$ and, furthermore, $\mathcal{L}_V(fW) = (\mathcal{L}_V f)W + f\mathcal{L}_V W$. Also note the following

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} (f \circ \Phi_t) &= (f' \circ \Phi_t) \frac{\partial \Phi_t}{\partial t} \\ &= Vf \circ \Phi_t \\ &= \mathcal{L}_V f \circ \Phi_t \, . \end{aligned} \tag{2.1}$$

The (smooth) assignment of a covector to each point of $U \subseteq M$ is called a **(differential) 1-form**, denoted by $\alpha(x) \in T_x^* M$. The set of all 1-forms in U is commonly denoted as $\Omega^1(U)$. The natural pairing $\langle \cdot, \cdot \rangle$ can be extended pointwise to the entire manifold and therefore to act on 1-forms and vector fields, $\langle \cdot, \cdot \rangle : \Omega^1(M) \times \mathfrak{X}(M) \to C^\infty(M, \mathbb{R})$. This allows us to write $vf = \langle \mathrm{d}f, v \rangle$ where, in local coordinates,

$$\mathrm{d}f = \frac{\partial f}{\partial x^i} \mathrm{d}x^i \in \Omega^1(M),$$

which is commonly referred to as the differential of f.

If we consider again a map $F : M \to N$, we can define the dual linear map $T_x^* F : T_{F(x)}^* N \to T_x^* M$ as

$$(T_x^* F(\alpha))(V) = \alpha(T_x F(V)), \quad \text{for } \alpha \in T_{F(x)}^* N, V \in T_x M. \tag{2.2}$$

If we have a 1-form $\alpha \in \Omega^1(M)$, then we can use the notation $T_x^* F(\alpha(F(x))) = (F^*\alpha)(x)$, and we say that $F^*\alpha$ is the **pullback** of α. Using the natural pairing, eq.(2.2) can be rewritten for vector fields and 1-forms as

$$\langle F^*\alpha, V \rangle (x) = \langle \alpha, F_* V \rangle (F(x)).$$

Note that using the pullback we can now generalize the relation (2.1) to

$$\frac{\mathrm{d}}{\mathrm{d}t} \Phi_t^* = \Phi_t^* \mathcal{L}_V \, ,$$

where again V is a vector field and Φ_t its associated flow.

The (smooth) assignment of a $\binom{p}{q}$-tensor gives rise to **tensor fields** of type $\binom{p}{q}$, denoted as $\mathcal{T}_q^p(M)$, and the point-wise extension of the tensor product leads to the tensor algebra, $\mathcal{T}(M)$. Analogously, the (smooth) assignment of a q-form gives rise to a (differential) q-form, and the set of these on M is denoted as $\Omega^q(M)$. The point-wise extension of the exterior product leads to the exterior algebra $\Omega^*(M)$.

Naturally, the interior product can be extended to the space of differential forms in similar fashion. However, working with differential forms allows us to introduce a new operation, the **exterior derivative**, $\mathrm{d} : \Omega^q(M) \to \Omega^{q+1}(M)$, which generalizes the notion of differential of a function. This operation can be defined as the unique map satisfying:

- $\mathrm{d}(a\alpha + b\beta) = a\mathrm{d}\alpha + b\mathrm{d}\beta$, for $\alpha, \beta \in \Omega^q(M)$ and $a, b \in \mathbb{R}$;
- d acting on $\Omega^0(M) \equiv C^\infty(M, \mathbb{R})$ is precisely the differential;
- $\mathrm{dd} = \mathrm{d}^2 = 0$;
- $\mathrm{d}(\alpha \wedge \omega) = \mathrm{d}\alpha \wedge \omega + (-1)^q(\alpha \wedge \mathrm{d}\omega)$, for $\alpha \in \Omega^q(M)$, $\omega \in \Omega^p(M)$.

Note that for $\Omega^0(M)$, the exterior product is nothing but the usual multiplication of a function.

One property that will be useful is that the exterior derivative commutes with pull-backs, that is,

$$F^*\mathrm{d}\alpha = \mathrm{d}\left(F^*\alpha\right)$$

We say that a form α is **closed** if $\mathrm{d}\alpha = 0$. If there exists a form β such that $\alpha = \mathrm{d}\beta$, then α is said to be **exact**. Clearly every exact form is closed by $\mathrm{d}^2 = 0$, but the converse is not necessarily true and it is dependent on the topology. The **Poincaré lemma** for smooth manifolds states that around any point on the manifold M there exists a neighborhood on which every closed form is exact.

It is worth mentioning an interesting identity, called *Cartan's magic formula*, which relates the exterior derivative and the interior product with the Lie derivative,

$$\mathcal{L}_V = \imath_V \mathrm{d} + \mathrm{d}\imath_V \qquad \text{(Cartan's magic formula)}$$

allowing us to compute the Lie derivative of a form easily.

Another interesting identity, this one relating only the interior product with the Lie derivative is

$$\imath_{\mathcal{L}_V W} = \mathcal{L}_V \imath_W - \imath_W \mathcal{L}_V,$$

which can be simplified using commutators as

$$\imath_{[V,W]} = \left[\mathcal{L}_V, \imath_W\right], \tag{2.3}$$

where the commutator on the right hand side is just operator notation [AM78].

2.1.2 Fibre bundles and vector bundles

A (smooth) **fibre bundle** over M with model fibre F is a (smooth) manifold E with projection $\pi : E \to M$ such that for every $x \in M$ there exists a neighborhood $U \subset M$ of x and a map $\Phi : \pi^{-1}(U) \subset E \to U \times F$, called a (smooth) local trivialization, such that Φ is a diffeomorphism. This implies the existence of adapted local coordinates for any point $p \in E$ of the form:

$$\Phi(p) = (x^1, ..., x^m, y^1, ..., y^k), \quad \text{with } k = \dim F,$$

where $x = \pi(p)$ has local coordinates $(x^1, ..., x^m)$, and $(y^1, ..., y^k)$ are the coordinates of a point in F. Clearly the dimension of E as a manifold is then $\dim M + \dim F = m + k$.

If it is possible to extend the trivialization to the entire base space M, then the bundle is said to be trivial. Otherwise, more than one trivialization will be required to cover it. Let (U_1, Φ_1) and (U_2, Φ_2) be two local trivializations such that $U_1 \cap U_2 \neq \emptyset$. Then there exists a smooth map $f_{12} : \pi^{-1}(U_1 \cap U_2) \subset E \to F$, called transition map or function, such that, with some abuse of notation:

$$\Phi_2 \circ \Phi_1^{-1}(p) = (\pi(p), f_{12}(p)).$$

A particular case of fibre bundle is where F is a k-dimensional vector space, in which case we refer to it as a **vector bundle** (of rank k). These will play a principal role in this work. For these, the transition functions simplify so that if $p \in \pi^{-1}(U_1 \cap U_2)$, such that $\Phi_1(p) = (x, v)$, then

$$\Phi_2 \circ \Phi_1^{-1}(p) = (x, f_{12}(p) \equiv g_{12}(x)v)$$

with $g_{12} : U_1 \cap U_2 \to GL(k, \mathbb{R})$, where $GL(k, \mathbb{R})$ is the general linear group of order k and we use matrix notation, gv, for the usual linear action of an element $g \in GL(k, \mathbb{R})$ on a vector v.

Given two vector bundles over M, $\pi : E \to M$, $\pi' : E' \to M$, of ranks k and k' respectively, one can generate a new vector bundle of rank $k + k'$, called the **Whitney sum** of E and E'. If $E_x = \pi^{-1}(x)$ and $E'_x = \pi'^{-1}(x)$ denote the respective fibres of each bundle at a point $x \in M$, the new bundle can be defined as $E \oplus E' = \bigsqcup_{x \in M}(E_x \oplus E'_x)$. Its projection $\pi_\oplus : E \oplus E' \to M$ and trivializations Φ are the obvious ones.

A (smooth) **section** of a bundle E is a smooth section of the projection π, i.e., $\sigma : U \subseteq M \to E$ such that $\pi \circ \sigma = \mathrm{Id}_U$. If the domain U can be extended to all of M, then the section is said to be a global section, otherwise it is said to be local. In the case of vector bundles there always exists at least a global section, the zero section $\zeta : M \to E$, $\zeta(x) = 0 \in E_x$. The space of all local sections from U is $\Gamma(U, E)$, and the space of global sections is usually denoted as $\Gamma(E) \equiv \Gamma(M, E)$. Clearly these spaces are vector spaces under pointwise addition and scalar multiplication,

$$(a\sigma + b\rho)(x) = a\sigma(x) + b\rho(x) \quad \text{with } \sigma, \rho \in \Gamma(U, E), a, b \in \mathbb{R}.$$

The latter can be easily extended to scalar multiplication with elements $f \in C^\infty(U, \mathbb{R})$, so $f\sigma \in \Gamma(U, E)$ is defined as

$$(f\sigma)(x) = f(x)\sigma(x).$$

The tangent bundle

A particular but very important case of vector bundle is the **tangent bundle** TM of a smooth manifold M. It is defined as the union of all the tangent spaces of M, that is,

$$TM = \bigsqcup_{x \in M} T_x M,$$

and comes equipped with the natural projection $\tau_M : TM \to M$, $z = (x, v) \mapsto x$ (we will frequently use the notation v_x to denote a point in TM but this may collide with labels from time to time). For us it will be of capital importance as this is the central stage of Lagrangian mechanics as the *velocity phase space* [see LR89; AM78].

The tangent bundle is itself a smooth manifold of dimension $2 \dim M = 2m$. We will commonly use the adapted local coordinates $(x^1, ..., x^m, v^1, ..., v^m)$.

This setting gives vector fields a new interpretation as sections of TM, i.e., $X : U \subseteq M \to TM$, with local coordinates

$$X(x) = (x^i, ..., x^m, X^1(x), ..., X^m(x)).$$

In fact, they are in one-to-one correspondence with each other.

If we have a smooth map $F : M \to N$, this defines a smooth global map $TF : TM \to TN$ by putting together all the different $T_xF : T_xM \to T_{F(x)}N$. This map is such that the following diagram commutes,

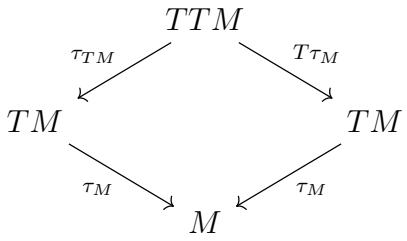
$$\begin{array}{ccc} TM & \xrightarrow{TF} & TN \\ {\scriptstyle \tau_M}\downarrow & & \downarrow{\scriptstyle \tau_N} \\ M & \xrightarrow{F} & N \end{array}$$

that is, $F \circ \tau_M = \tau_N \circ TF$. TF is a *vector bundle morphism*, meaning that it maps fibres into fibres and it does so linearly, which is immediately apparent due to the linearity of T_xF for each x. In adapted local coordinates we have:

$$TF(x^1, ..., x^m, v^1, ..., v^m) = \left(F^1(x), ..., F^n(x), \frac{\partial F^1(x)}{\partial x^i} v^i, ..., \frac{\partial F^n(x)}{\partial x^i} v^i \right).$$

Note also that if F and G are two maps such that $F \circ G$ is well-defined, then $T(F \circ G) = TF \circ TG$.

Of course, the notion of tangent bundle of a tangent bundle is well defined, as TM is itself a smooth manifold. The construction can be stacked further, but for the remainder of the section it will be sufficient to consider TTM in relation with TM. The bundle $\tau_{TM} : TTM \to TM$ is also a vector bundle of rank $2m$ over TM. Note that $T_z\tau_M : T_zTM \to T_{\tau_M(z)}M = T_xM$, and this defines a global map $T\tau_M : TTM \to TM$ such that the following diagram commutes:



If we denote a point in TTM using local adapted coordinates (x, v, X_x, X_v), we have that $\tau_{TM}(x, v, X_x, X_v) = (x, v)$ and $T\tau_M(x, v, X_x, X_v) = (x, X_x)$.

Let us then consider the n-dimensional vector subspace $V_zTM = \ker T_z\tau_M \subset T_zTM$. The union of all these subspaces over TM,

$$VTM = \bigsqcup_{z \in TM} V_zTM,$$

is a vector bundle of rank m over TM which we call the **vertical bundle**. If a vector field $X \in \mathfrak{X}(TM)$ defines a section in VTM, then the vector field is said to be *vertical*.

Now, with this structure in place, we can tackle some of the canonical operations and objects that are available in any tangent bundle.

If $\gamma : I \subseteq \mathbb{R} \to M$ is a smooth curve, then we define its **tangent (or natural) lift** as the curve $\hat{\gamma} : I \subseteq \mathbb{R} \to TM$, $t \mapsto (\gamma(t), \dot{\gamma}(t))$. Clearly $\tau_M \circ \hat{\gamma} = \gamma$.

If $u \in T_xM$, $x \in M$, we define its **vertical lift** as the vector $u^v \in V_zTM \subset T_zTM$, $z = (x, v) \in TM$ which results in the tangent vector at $t = 0$ of the curve $\sigma : I \subseteq \mathbb{R} \to TM$, $t \mapsto (x, v + tu)$, that is,

$$u^v(x, v) = \left. \frac{\mathrm{d}}{\mathrm{d}t} \right|_{t=0} (x, v + tu)$$

This notion can be extended to vector fields, so if $X \in \mathfrak{X}(M)$, then $X^v \in \mathfrak{X}(TM)$ such that $X^v(z) = (X(\tau_M(z)))^v$ which defines a section of VTM. In adapted local coordinates this vector field takes the form

$$X^v(x, v) = X^i(x) \partial_{v^i}.$$

The vertical lift operation is linear, that is, for $f \in C^\infty(M,\mathbb{R})$ and $X, Y \in \mathfrak{X}(M)$, $(X + fY)^v = X^v + (f \circ \tau_M)Y^v$.

If $f : M \to \mathbb{R}$ is a smooth function on M, that is, $f \in C^\infty(M,\mathbb{R})$, then its **complete lift**, $f^c : TM \to \mathbb{R}$ is defined by

$$f^c(x,v) = (T_x f)v = v(x)f$$

If $X \in \mathfrak{X}(M)$ is a smooth vector field on M with local presentation $X(x) = X^i(x)\partial_{x^i}$ and $\Phi_t : M \to M$ is its associated local flow, then $T\Phi_t : TM \to TM$ is again a flow whose infinitesimal generator $X^c \in \mathfrak{X}(TM)$ is what we call **complete lift** of X. In adapted local coordinates this takes the form

$$X^c(x,v) = X^i(x)\partial_{x^i} + v^j \frac{\partial X^i}{\partial x^j}(x)\partial_{v^i}$$

There is also a particularly important class of vector fields on TM called **semisprays on** M (also known as *second order differential equation vector fields* or its acronym *SODE*). These are vector fields on TM such that they are sections of both $\tau_{TM} : TTM \to TM$ and $T\tau_M : TTM \to TM$. This implies that if Y is a smooth semispray on M, then in local coordinates it shall take the form

$$Y(x,v) = v^i\partial_{x^i} + Y^i(x,v)\partial_{v^i},$$

with $Y^i(x,v)$ smooth.

Finally, let us define two important canonical objects on the tangent bundle. The first is the so-called **Liouville vector field** (also *canonical vector field*), which we will denote as $\triangle$. This vector field can be defined as the infinitesimal generator of the flow $\Phi_t : TM \to TM$, $(x,v) \mapsto (x, e^t v)$, from which it is clear that this is a vertical vector field. In local coordinates it takes the simple form

$$\triangle(x,v) = v^i\partial_{v^i}.$$

The second object is the **canonical endomorphism** $S : TTM \to TTM$, a vector bundle morphism such that $\mathrm{im}S = \ker S = VTM$. Therefore, it satisfies that $S^2 = S \circ S = 0$. We may define it by

$$S(X(z)) = (T\tau_M(X(z)))^v,$$

and it can be regarded as a $\binom{1}{1}$ tensor field on M, which in adapted local coordinates has the form

$$S = \partial_{v^i} \otimes \mathrm{d}x^i.$$

Given $Z \in TM$ with coordinates (x, v, Z_x, Z_v), then

$$S(x, v, Z_x, Z_v) = (x, v, 0, Z_x).$$

It can be checked that if $X \in \mathfrak{X}(M)$, then

$$S(X^c) = X^v\,.$$

Using this, it is not difficult to check that if Y is a semispray, then $S(Y) = \triangle$, which also serves to characterize these.

Another property of S that will be used later on is the following. Given $X, Y \in \mathfrak{X}(TM)$, then

$$[S(X), S(Y)] = S([S(X), Y]) + S([X, S(Y)]) \tag{2.4}$$

We define the adjoint operator of the canonical endomorphism, S^*, by the relations

$$S^*(f) = f\,, \quad \text{for } f \in C^\infty(TM)$$
$$(S^*(\alpha))(X_1, ..., X_p) = \alpha(S(X_1), ..., S(X_p))\,, \quad \text{for } \alpha \in \Omega^p(TM)$$

Locally this implies that

$$S^*(\mathrm{d}x^i) = 0 \quad S^*(\mathrm{d}v^i) = \mathrm{d}x^i$$

This adjoint operator serves to characterize a special subset of p-forms on TM which will appear frequently in this work. If $\alpha \in \Omega^p(TM)$ such that $\alpha \in \mathrm{im}S^*$, then it is said to be **semibasic**. This means that, locally, it can be spanned by

$$\left\{\mathrm{d}x^{i_1} \wedge ... \wedge \mathrm{d}x^{i_p}, 1 \leq i_1 < ... < i_p \leq m\right\}$$

In particular, if $\beta \in \Omega^1(TM)$ is semibasic, it will have a local presentation

$$\beta = \beta_i(x, v)\mathrm{d}x^i\,.$$

To end this section, let us introduce a type of maps between TM and M which will be useful for us in several parts of this work.

Definition 2.1.1. A smooth map $R : TM \to M$ is a **tangent retraction** or simply a retraction on M [see AMS08, chapter 4] if it satisfies the following properties. If we denote by $R_x = R|_{T_xM}$ the restriction of R to T_xM, then:

- $R_x(x, 0) = x$,
- Identifying $T_{(x,0)}T_xM \cong T_xM$ then $T_{(x,0)}R_x = \mathrm{Id}_{T_xM}$.

With such a map, for a given point $(x, v) \in TM$ we may generate a curve $\gamma_v : [0, 1] \to M, t \mapsto R(x, tv)$ such that $\gamma_v(0) = x$ and $\dot\gamma(t) = v$. The point $\gamma_v(1) = R(x, v)$ can be thought of as a translation of x along the curve, which generalizes the concept of *translation* from affine and Euclidean geometry.

Given a vector field on M, it naturally generates a retraction map via its associated flow, and the retraction just moves a given point along the integral curve passing through it, which serves as a generalization of the above example. Also, if our manifold were endowed with a Riemannian structure, which we will not study here, the concept of a geodesic can be used to generate a retraction.

The cotangent bundle and symplectic manifolds

Another very important vector bundle in mechanics is the **cotangent bundle** T^*M of a smooth manifold M [see LR89]. The cotangent bundle is a smooth manifold of dimension $2\dim M = 2m$ and it is defined as the union of all the cotangent spaces of M, that is,

$$T^*M = \bigsqcup_{x \in M} T^*_xM.$$

It comes equipped with the natural projection $\pi_M : T^*M \to M$, $\zeta = (x, p) \mapsto x$.

Similar to what happened in the tangent bundle, if we have a smooth map $F : M \to N$, this defines a smooth global map $T^*F : T^*N \to T^*M$ as $T^*_xF : T^*_{F(x)}N \to T^*_xM$. This map is such that the following diagram commutes,

$$\begin{array}{ccc} T^*M & \xleftarrow{T^*F} & T^*N|_{F(M)} \\ {\scriptstyle \pi_M}\downarrow & & \downarrow{\scriptstyle \pi_N} \\ M & \xrightarrow{\quad F \quad} & N \end{array}$$

that is, $F \circ \tau_M \circ T^*F = \tau_N$. T^*F is a *vector bundle morphism*. Note also that if F and G are two maps such that $F \circ G$ is well-defined, then $T^*(F \circ G) = T^*G \circ T^*F$.

The cotangent bundle will be the central stage of Hamiltonian mechanics and the most obvious point of connection between mechanics and geometry due to its intrinsic geometric structure, the *symplectic structure*. Before proceeding, let us talk briefly about what a symplectic vector space is.

Definition 2.1.2. Let V be a $2m$-dimensional vector space equipped with a characteristic 2-form ω. If ω is non-degenerate, i.e. $\ker \omega = 0 \Leftrightarrow \bigwedge_{i=1}^{m} \omega \equiv \omega^m \neq 0$, we say it is a *symplectic structure* for V. The pair (V, ω) is then a **symplectic vector space**.

Consider now the dual vector space associated to V, denoted by V^*. Let us define the following linear map between V and V^*:

$$\begin{aligned} \flat_\omega : V &\to V^* \\ v &\mapsto \flat_\omega(v) = \imath_v \omega \end{aligned}$$

If (V, ω) is a symplectic vector space, then this map is a linear isomorphism of vector spaces. Its inverse is commonly denoted as $\sharp_\omega \equiv \flat_\omega^{-1}$ and both are referred to as *musical isomorphisms*.

Additionally, if (V, ω) is a symplectic vector space, there exists a basis $\{e_i\}_{i=1}^{2m}$ which satisfies $\forall i, j = 1, ..., m$:

- $\omega(e_i, e_{j+m}) = -\omega(e_{j+n}, e_i) = \delta_{ij}$,
- $\omega(e_i, e_j) = \omega(e_{i+n}, e_{j+m}) = 0$.

where δ_{ij} is the Kronecker delta defined as:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

The characteristic 2-form provides us with a notion of orthogonality. If $U \subset V$ is a vector subspace then, its ω-*orthogonal* (or *symplectic complement*), $U^\perp$, is the space

$$U^\perp = \{u \in V \,|\, \omega(u, u') = 0, \, \forall u' \in U\}.$$

Definition 2.1.3. A vector subspace U of a symplectic vector space (V, ω) is called:

- **isotropic** if $U \subset U^\perp$, i.e., $\omega(u, u') = 0$, $\forall u, u' \in U$.
- **coisotropic** if $U^\perp \subset U$, i.e., $\omega(u, u') = 0$, $\forall u, u' \in U^\perp$.
- **symplectic** if $(U, \omega|_U)$ is a symplectic vector space, i.e., $\omega|_U \neq 0$. Equivalently, $U \cap U^\perp = \{0\}$.
- **Lagrangian** if U is both isotropic and coisotropic ($U = U^\perp$).

Intuitively, the manifold extension of the concept of a symplectic vector space is naturally that of a manifold whose tangent spaces are symplectic vector spaces.

Definition 2.1.4. Let S be a $2m$-dimensional smooth manifold. S is said to be a **symplectic manifold** if there exists a non-degenerate 2-form $\omega \in \Omega^2(S)$ such that each pair $(T_\zeta S, \omega_\zeta), \forall \zeta \in S$ is a symplectic vector space, together with the additional condition of being closed, i.e. $\mathrm{d}\omega = 0$.

We say that a vector field $X \in \mathfrak{X}(S)$ is symplectic if and only if

$$\mathcal{L}_X \omega = 0.$$

By Cartan's magic formula this is equivalent to $\imath_X \omega$ being a closed form. This also implies that if Φ_t is the (local) flow induced by X, then

$$\Phi_t^* \omega = \omega,$$

as we know that

$$\frac{\mathrm{d}}{\mathrm{d}t} \Phi_t^* \omega = \Phi_t^* \mathcal{L}_X \omega,$$

Then Φ_t is said to be a (local) symplectomorphism.

If X, Y are two symplectic vector fields on S, then applying the identity in eq.(2.3), we get that its commutator then satisfies

$$\imath_{[X,Y]} \omega = -\mathrm{d}\left(\omega(X, Y)\right)$$

Analogous to the vector space case we can also define a map, this time a linear vector bundle homomorphism, $\flat_\omega : TS \to T^*S$, where TS and T^*S are respectively the tangent and cotangent bundles of S. Owing to the non-degeneracy condition, this mapping can be shown to be a vector bundle isomorphism. As in the vector space case, its inverse is commonly denoted as $\sharp_\omega : T^*S \to TS$.

To each function $f \in C^k(S, \mathbb{R})$, with $k \geq 1$, we can associate a vector field $X_f \in \mathfrak{X}(S)$ called a **Hamiltonian vector field**, defined by:

$$\imath_{X_f} \omega = \mathrm{d}f.$$

Note that every Hamiltonian vector field is symplectic, which is easy to see applying Cartan's magic formula:

$$\begin{aligned} \mathcal{L}_{X_f} \omega &= \imath_{X_f} \mathrm{d}\omega + \mathrm{d}\left(\imath_{X_f} \omega\right) \\ &= \mathrm{d}\mathrm{d}f \\ &= 0. \end{aligned}$$

Also note that by eq.(2.1.2), the commutator of two symplectic vector fields X and Y is itself the Hamiltonian vector field of the function $-\omega(X, Y)$.

According to the Darboux theorem, if (S, ω) is a symplectic manifold, then for each point $\zeta \in S$ there exists a neighborhood $\phi_\zeta : U_\zeta \to \mathbb{R}^{2m}$ inducing local coordinates $(x^1, ..., x^m, p_1, ..., p_m)$ such that the symplectic form can be written as

$$\omega = \mathrm{d}x^i \wedge \mathrm{d}p_i. \tag{2.5}$$

One can also classify a submanifold K of a symplectic manifold (S, ω) in analogy to the subspaces of a symplectic vector space case:

- **isotropic** if $T_xK \subset (T_xK)^\perp$.
- **coisotropic** if $(T_xK)^\perp \subset T_xK$.
- **symplectic** if $(K, \omega|_K)$ is a symplectic manifold. Equivalently, $(T_xK) \cap (T_xK)^\perp = \{0\}$.
- **Lagrangian** if $T_xK = (T_xK)^\perp$, $\forall x \in K$.

Every cotangent bundle T^*M is itself a symplectic manifold, and in fact the very concept spanned from this example. The adapted local coordinates are precisely those of the Darboux theorem. To see this, let us first introduce another canonical object.

Let $V \in \mathfrak{X}(T^*M)$ and consider the 1-form $\theta \in \Omega^1(T^*M)$ defined pointwise by

$$\theta_{(x,p)}(V) = p\left(\left(T_{(x,p)}\pi\right)V\right).$$

This is called the **canonical 1-form** (or *tautological 1-form*) and using adapted local coordinates it can be written as

$$\theta = p_i \mathrm{d}x^i.$$

It can be immediately seen that the 2-form $\omega = -\mathrm{d}\theta$ is a symplectic form which in adapted local coordinates is expressed precisely as in eq.(2.5).

Poisson brackets and Poisson manifolds

If $f, g \in C^k(S, \mathbb{R})$, $k \geq 1$, and $X_f, X_g \in \mathfrak{X}(S)$ are their associated Hamiltonian vector fields we can define a $\mathbb{R}$-bilinear operation $\{\cdot,\cdot\} : C^\infty(S,\mathbb{R}) \times C^\infty(S,\mathbb{R}) \to C^\infty(S,\mathbb{R})$ called Poisson bracket by

$$\{f, g\} = \omega(X_f, X_g)$$

Satisfying:

- Anti-symmetry: $\{f, g\} = -\{g, f\}$
- Leibniz product: $\{fh, g\} = \{f, g\}\, h + f\, \{h, g\}$
- Jacobi identity: $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$

This endows the space $C^\infty(S, \mathbb{R})$ with a Lie algebra structure.

In this space there may be distinguished elements $c \in C^\infty(S, \mathbb{R})$ that satisfy

$$\{c, f\} = 0, \quad \forall f \in C^\infty(S, \mathbb{R}).$$

These are called **Casimir elements** (or *Casimir functions*) of the Poisson structure [see MR99].

With the Poisson bracket we can write

$$X_f(g) = \{g, f\},$$

and we can also give yet another interpretation to eq.(2.1.2) as

$$[X_f, X_g] = -X_{\{f,g\}}.$$

If P is a smooth manifold equipped with a bracket on $C^\infty(P,\mathbb{R})$ satisfying the properties above, then $(P,\{\cdot,\cdot\})$ is said to be a Poisson manifold. This implies that every symplectic manifold S is a Poisson manifold, but the converse is not true.

Note that in any Poisson manifold we can define an object $\Pi : T^*P \times T^*P \to \mathbb{R}$, by the relation

$$\{f,g\} = \Pi(\mathrm{d}f, \mathrm{d}g)$$

This object is called the **Poisson bivector field**. It is a $\binom{2}{0}$ antisymmetric tensor field. Using it we can define a map, $\sharp^\Pi : T^*P \to TP$, $\mu = \sharp^\Pi(\mu) = \Pi(\cdot,\mu)$. Thus

$$X_h = \sharp^\Pi(\mathrm{d}h)$$

In the particular case where P is a symplectic manifold with symplectic form ω, then we have that the bivector and the symplectic form are related by $\Pi = \omega^{-1}$, and from the Darboux theorem, it takes the local form:

$$\Pi = \partial_{x^i} \wedge \partial_{p_i},$$

where the wedge indicates an antisymmetric tensor product.

Tulczyjew's triple

Let TTM, T^*TM, TT^*M and T^*T^*M be the double bundles derived from the tangent and cotangent bundles. The Tulczyjew's triple is an isomorphic relation between the latter three bundles just mentioned, via two isomorphisms $\alpha_M : TT^*M \to T^*TM$ and $\beta_M : TT^*M \to T^*T^*M$ introduced in his papers [Tul76a; Tul76b].

In order to construct the first isomorphism let us define the canonical involution [see God69], $\kappa_M : TTM \to TTM$, as the map such that for all $f \in C^\infty(\mathbb{R}^2, M)$,

$$\kappa_M\left(\frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0}\left(\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} f(t,s)\right)\right) = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\left(\frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} f(t,s)\right).$$

In adapted local coordinates we have that $\kappa_M(x,v,X_x,X_v) = (x,X_x,v,X_v)$.

Next, let us define the pairing $\langle\!\langle\cdot,\cdot\rangle\!\rangle : TT^*M \times_M TTM$ as

$$\left\langle\!\!\left\langle \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\alpha(t), \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} v(t)\right\rangle\!\!\right\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\langle\alpha(t), v(t)\rangle,$$

with $\alpha \in C^\infty(\mathbb{R}, T^*M)$ and $v \in C^\infty(\mathbb{R}, TM)$ such that $\pi_M(\alpha(t)) = \tau_M(x(t))$.

Using these elements we can finally define α_M as the map defined by the relation

$$\langle\alpha_M(W), V\rangle_{TM} = \langle\!\langle W, \kappa_M(V)\rangle\!\rangle,$$

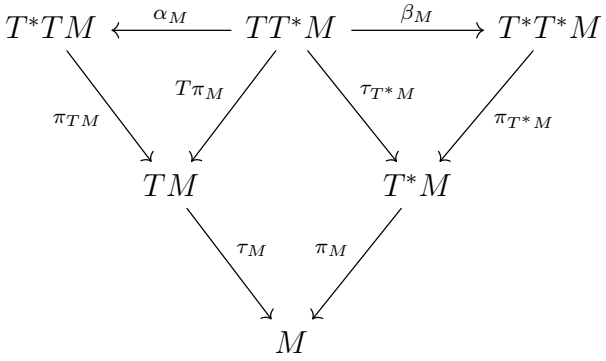
where $W \in TT^*M$, $V \in TTM$.

The second isomorphism, β_M, is much easier to define, as it is nothing but

$$\beta_M(V) = \flat_\omega(V),$$

where $V \in TT^*M$ and ω is the canonical symplectic 2-form of T^*M.

If we let $\pi_{TM} : T^*TM \to TM$, $\pi_{T^*M} : T^*T^*M \to T^*M$ and $\tau_{T^*M} : TT^*M \to T^*M$ denote the projections that play a role in the construction, then the following diagram commutes:



Let U be a neighborhood of M so that $U_{T^*TM} \equiv \pi_{TM}^{-1}\left(\tau_M^{-1}(U)\right) \subset T^*TM$, $U_{TT^*M} \equiv \tau_{T^*M}^{-1}\left(\pi_M^{-1}(U)\right) \subset TT^*M$ and $U_{T^*T^*M} \equiv \pi_{T^*M}^{-1}\left(\pi_M^{-1}(U)\right) \subset T^*T^*M$. Assuming local coordinates on $U_{T^*TM} : (x, v, p_x, p_v)$, $U_{T^*T^*M} : (y, p_y, \varpi_y, \varpi_{p_y})$ and $U_{TT^*M} : (z, \zeta, v_z, v_\zeta)$ such that $x = y = z$, Tulczyjew's isomorphisms α_M and β_M take the forms

$$\alpha_M(z, \zeta, v_z, v_\zeta) = (z, v_z, v_\zeta, \zeta),$$
$$\beta_M(z, \zeta, v_z, v_\zeta) = (z, \zeta, -v_\zeta, v_z).$$

Thus, α_M maps $(x = z, v = v_z, p_x = v_\zeta, p_v = \zeta)$, and β_M maps $(y = z, p_y = \zeta, \varpi_y = -v_\zeta, \varpi_{p_y} = v_z)$.

The double bundles T^*TM and T^*T^*M have canonical symplectic structures ω_{TM} and ω_{T^*M} respectively, generated from their corresponding tautological 1-forms ω_{TM} and ω_{T^*M}. In the adapted local coordinates used above these take the form

$$\theta_{TM} = p_{x^i}\mathrm{d}x^i + p_{v^i}\mathrm{d}v^i$$
$$\theta_{T^*M} = \varpi_{y^i}\mathrm{d}y^i + \varpi_{p_i}\mathrm{d}p_i$$
$$\omega_{TM} = \mathrm{d}x^i \wedge \mathrm{d}p_{x^i} + \mathrm{d}v^i \wedge \mathrm{d}p_{v^i}$$
$$\omega_{T^*M} = \mathrm{d}y^i \wedge \mathrm{d}\varpi_{y^i} + \mathrm{d}p_i \wedge \mathrm{d}\varpi_{p_i}$$

The isomorphisms α_M, β_M are symplectomorphisms (more precisely β_M is an antisymplectomorphism), and defining two symplectic structures in TT^*M by $\omega_\alpha = \alpha_M^*\omega_{TM}$ and $\omega_\beta = \beta_M^*\omega_{T^*M}$. As it turns out, $\omega_\alpha = -\omega_\beta$ and in local coordinates

$$\omega_\alpha = \mathrm{d}z^i \wedge \mathrm{d}v_{\zeta_i} + \mathrm{d}v_{z^i} \wedge \mathrm{d}\zeta_i\,.$$

This can also be defined as the complete lift of ω_M to TT^*M.

Higher order tangent bundles

Let us briefly mention the concept of higher order tangent bundles. The idea is a generalization of the construction used for the tangent bundle [see LR85].

Consider a smooth curve $\gamma : I \subset \mathbb{R} \to M$ that passes through $x \in M$, such that $\gamma(0) = x$ for some $0 \in I$. Given two such curves γ_1 and γ_2 passing through x, we say that they have a tangency of order $s \geq 1$ at x if there exists a chart (U, ϕ) with $x \in U$, such that

$$\frac{\mathrm{d}^k}{\mathrm{d}t^k}(\phi \circ \gamma_1)(t)\bigg|_{t=0} = \frac{\mathrm{d}^k}{\mathrm{d}t^k}(\phi \circ \gamma_2)(t)\bigg|_{t=0}, \quad \text{for } k = 0, ..., s$$

This generates a new equivalence class $[\gamma]^{(s)}$ at x. The set of all these equivalence classes at x conforms the **tangent space of order *s*** of M at x, denoted by $T_x^{(s)}M$. The disjoint

union of all these spaces conforms the tangent bundle of order s, $T^{(s)}M$, which is a smooth manifold of dimension $(s+1)m$ and, together with the projection $\tau_M^{(s)} : T^{(s)}M \to M$, it is a fibre bundle over M. It is clear that when $s = 1$, $T^{(1)}M = TM$.

There is a canonical inclusion, $i_s : T^{(s)}M \hookrightarrow TT^{(s-1)}M$ defined as $i_k\left([\gamma]^{(s)}\right) = [\hat{\gamma}^{(s-1)}]^{(1)}$, where $\hat{\gamma}^{(k)} : I \subseteq \mathrm{R} \to T^{(k)}M$ is the **tangent lift of order** k. In local coordinates, $\gamma(t) = (\gamma^1(t), ..., \gamma^m(t))$, this reads

$$i_s(\gamma(t), \dot{\gamma}(t), ..., \gamma^{(s)}) = (\gamma(t), \dot{\gamma}(t), ..., \gamma^{(s-1)}(t), \dot{\gamma}(t), ..., \gamma^{(s-1)}(t), \gamma^{(s)}(t))$$

2.1.3 Lie groups and Lie groupoids

Lie groups and actions

A **Lie group** G is both a smooth manifold and an algebraic group whose operations are smooth. This means that they are equipped with a smooth and associative multiplication map, $\mu : G \times G \to G$, and a smooth inversion map $\iota : G \to G$, and that there exists an identity element, e, so that

$$\begin{aligned} \mu(g, e) = \mu(e, g) = g, \quad \forall g \in G \\ \mu(g, \iota(g)) = \mu(\iota(g), g) = e. \end{aligned}$$

Some of the most salient examples of Lie groups are matrix Lie groups, such as the *general linear group* of order n,

$$GL(n, \mathbb{R}) = \{A \in M_n(\mathbb{R}) \mid \det A \neq 0\},$$

which is an n^2-dimensional manifold, or the *special orthogonal group* (rotations) of order n,

$$SO(n) \equiv SO(n, \mathbb{R}) = \left\{A \in GL(n, \mathbb{R}) \,|\, A^T A = A A^T = I_n\right\},$$

which is itself a subgroup (and submanifold) of $GL(n, \mathbb{R})$. As in these groups the group operation is simply matrix multiplication, it is common to introduce *matrix notation* where the multiplication map becomes simple yuxtaposition, and inversion is denoted as $(\cdot)^{-1}$, that is,

$$\begin{aligned} \mu(g, h) = gh, \quad \forall g, h \in G \\ \iota(g) = g^{-1}, \end{aligned}$$

which simplifies the notation substantially in some cases.

Given $h \in G$ we can define three different automorphisms from the multiplication operation

$$\begin{aligned} L_h &: G \to G, \qquad g \mapsto hg, \\ R_h &: G \to G, \qquad g \mapsto gh, \\ C_h &: G \to G, \qquad g \mapsto hgh^{-1}, \end{aligned}$$

the first two called **left** and **right translation** respectively, and the third is called **conjugation**. Here identities such as $C_h = L_h \circ R_{h^{-1}}$, $L_{gh} = L_g \circ L_h$, $R_{gh} = R_h \circ R_g$ or $L_g^{-1} = L_{g^{-1}}$ hold true.

These operations can be thought of as the group G acting on itself. In a similar manner, we can generalize this situation to have a smooth manifold M and a Lie group

G that acts on it. We say that an action of the Lie group G on M is a smooth map $\phi : G \times M \to M$ such that,

$$\phi(e, x) \equiv \phi_e x = x.$$

ϕ is said to be a **left action** if for any two elements $g, h \in G$,

$$\phi_g \phi_h x = \phi_{gh} x = ghx,$$

and **right action** if

$$\phi_g \phi_h x = \phi_{hg} x = xhg.$$

We call the set

$$\mathcal{O}_x = \{\phi^x(g) \in M \,|\, g \in G\} \subset M$$

the **orbit** of x, and the set

$$G_x = \{g \in G \,|\, \phi_g(x) = x\} \subset G$$

the **isotropy group** (or *stabilizer*) of x, which is indeed a Lie subgroup.

An action is said to be

- **transitive** if for every pair $x, y \in M$ there exists $g \in G$ such that $\phi_g(x) = y$, or equivalently, if there is only a single orbit which is M itself;
- **faithful** (or *effective*) if the map $\phi^x : G \to M$ is injective;
- **free** if the isotropy group of every point $x \in M$ is trivial, that is, it only contains the identity.

Note that every free action is faithful [see MR99; AM78].

Under certain conditions about the action, namely that it be free and *proper* in the topological sense, it is possible to guarantee that the set of all distinct orbits, M/G, is a smooth manifold, and the map $\pi : M \to M/G$, $x \mapsto \mathcal{O}_x$ is a smooth submersion (that is, a projection) [see AM78, theorem 4.1.20].

If instead of M/G we consider G/H with $H \subset G$ a closed Lie subgroup, this is always a smooth submanifold [see AM78, corollary 4.1.21].

If we have a map $F : M \to N$ and two actions $\phi : G \times M \to M$, $\psi : G \times N \to N$, the map F is said to be **equivariant** (with respect to these actions of G) if

$$F(\phi_g x) = \psi_g F(x) \quad \forall g \in G,$$

that is, if the following diagram commutes for each $g \in G$

$$\begin{array}{ccc} M & \xrightarrow{F} & N \\ {\scriptstyle \phi_g}\downarrow & & \downarrow{\scriptstyle \psi_g} \\ M & \xrightarrow{F} & N \end{array}$$

This will be important in mechanics, as these notions translate into symmetries of a mechanical system and these in turn lead to conserved quantities through Noether's theorem.

Vector fields on a Lie group and Lie algebras

As in any other smooth manifold, it makes sense to talk about the tangent (and cotangent) space of G at a point g, T_gG (T_g^*G). Consequently, the notions of vector field, 1-form and tensor field extend to Lie groups.

On a (finite dimensional) Lie group G there is a set of special vector fields, called **left-invariant** (resp. **right-invariant**) vector fields. These are those fields $X \in \mathfrak{X}(G)$ that satisfy the relation

$$(T_hL_g)\,X(h) = X(gh) \quad (\text{resp. } (T_hR_g)\,X(h) = X(hg)),$$

for all $g, h \in G$. Since translations are diffeomorphisms, then we may just write $(L_g)_*X = X$ (resp. $(R_g)_*X = X$). Note that given a vector $X_e \in T_eG$, this defines a left-invariant (resp. right-invariant) vector field on G by translation which we may denote as $\overleftarrow{X} = (L_g)_*X_e$ (resp. $\overrightarrow{X} = (R_g)_*X_e$). These vector fields form a linear subspace of $\mathfrak{X}(G)$, and, furthermore, they are closed under Lie brackets, i.e.,

$$\begin{aligned}(L_g)_*[X,Y] &= [(L_g)_*X, (L_g)_*Y] = [X,Y] \\ &\text{(resp. } (R_g)_*[X,Y] = -[(R_g)_*X, (R_g)_*Y] = [X,Y]).\end{aligned}$$

Any vector space V equipped with a bilinear multiplication operation forms an algebra. If this multiplication, which we conveniently note as $[\cdot,\cdot] : V \times V \to V$, further satisfies

- antisymmetry: $[X,Y] = -[Y,X]$,
- Jacobi identity: $[X,[Y,Z]] + [Y,[Z,X]] + [Z,[X,Y]] = 0$,

for all $X, Y, Z \in V$, then $(V, [\cdot,\cdot])$ forms a **Lie algebra**. If $U \subseteq V$ is closed under the bracket operation, then $(U, [\cdot,\cdot]|_U)$ is a Lie subalgebra.

$\mathfrak{X}(G)$ is a Lie algebra under the Lie bracket, and the set of left-invariant vector fields is a Lie subalgebra (as is the set of right-invariant vector fields), which we denote as $\mathfrak{g}$. It can be shown that the latter is a finite dimensional vector space of the same dimension as G, and in fact can be set in isomorphic relation with the tangent space of G at e, that is, $\mathfrak{g} \cong T_eG$.

$\mathfrak{g}$ being a vector space, we may choose a basis in $\mathfrak{g}$, say $\{e_a\}_{a=1}^n$, with $n = \dim \mathfrak{g}$. If we compute the bracket of the elements of the basis, we get relations of the form

$$[e_a, e_b] = C_{ab}^d e_d, \quad \text{for } a, b = 1, ..., n.$$

The coefficients C_{ab}^d are called the **structure constants** of the Lie algebra.

An element ξ of the Lie algebra is in a one-to-one correspondence with a left-invariant vector field on G. If γ_ξ denotes the 1-parameter (sub)group generated by the left-invariant vector field associated with ξ, then γ_ξ defines a curve on G such that $\gamma_\xi(0) = e$. From this we can generate a map between the algebra and the group called the **exponential map**, $\exp : \mathfrak{g} \to G$, by

$$\exp(\xi) = \gamma_\xi(1).$$

In the case of matrix Lie groups this map coincides with the usual definition of the matrix exponential, hence the name. This map is smooth and such that $T_0 \exp = \mathrm{Id}_{\mathfrak{g}}$ and so it can be regarded as a retraction on G restricted to $T_eG \cong \mathfrak{g}$. Note that $\exp(t\xi) = \gamma_{t\xi}(1) = \gamma_\xi(t)$, which we will use frequently, and also that $\exp(-\xi) = (\exp(\xi))^{-1}$.

Furthermore it is always possible to find neighborhoods of $0 \in \mathfrak{g}$, $\mathfrak{u}_0$, and $e \in G$, U_e, so that $\exp|_{\mathfrak{u}_0} : \mathfrak{u}_0 \to U_e$ is a diffeomorphism.

If we consider the map $C : G \times G \to G$, $(h, g) \mapsto C_h(g) = hgh^{-1}$, this can be interpreted as an action of the group G on itself. From it we can derive the action of G on its Lie algebra $\mathfrak{g}$, the **adjoint action** $\mathrm{Ad} : G \times \mathfrak{g} \to \mathfrak{g}$, by differentiation. If $g = \exp(\xi)$, then

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} C_h(\exp(t\xi)) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} h\exp(t\xi)h^{-1} = (T_eC_h)\,\xi = \mathrm{Ad}_h\xi$$

We may also obtain the action of the algebra on itself, the **adjoint operation** $\mathrm{ad} : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ in a similar fashion, if $h = \exp(\eta)$,

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathrm{Ad}_{\exp(t\eta)}\xi &= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \exp(t\eta)\xi\exp(t\eta)^{-1} \\ &= \eta\xi - \xi\eta = [\eta, \xi] = \mathrm{ad}_\eta\xi\end{aligned}$$

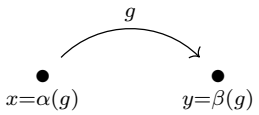
Lie groupoids

It is possible to generalize the concept of group to that of a groupoid by allowing the multiplication operation to be a partial map, that is, such that not every element can be multiplied by every other element. In a similar fashion it is possible to generalize the concept of a Lie group and Lie algebra to that of Lie groupoid and Lie algebroid [see Wei96a; Mac87; Mac05].

The former will play a particular role in part of this thesis but they are both a recurrent theme in the study of the relation between what we call continuous and discrete mechanics [see Wei96b]. Let us first recall what a groupoid is.

Definition 2.1.5. A **groupoid** over a set M is a set G together with the following *structural maps*:

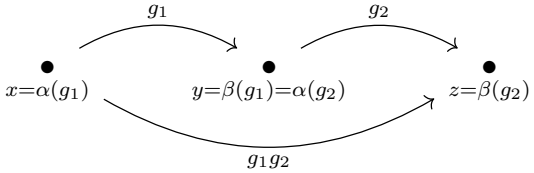
- A pair of maps $\alpha, \beta : G \to M$, the *source* and *target*. This allows us to think of an element $g \in G$ as an arrow from $x = \alpha(g)$ to $y = \beta(g)$ in M



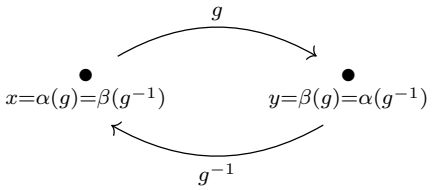
  The source and target maps define the set of *composable pairs*

$$G_2 = \{(g_1, g_2) \in G \times G \,|\, \beta(g_1) = \alpha(g_2)\}\,.$$

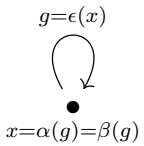
- A *multiplication* on composable elements $\mu : G_2 \to G$, denoted simply by $\mu(g_1, g_2) = g_1g_2$ using matrix notation, such that
  - $\alpha(g_1g_2) = \alpha(g_1)$ and $\beta(g_1g_2) = \beta(g_2)$.
  - $g_1(g_2g_3) = (g_1g_2)g_3$.



- An *inversion* map $\iota : G \to G$, denoted simply by $\iota(g) = g^{-1}$, such that
  - $g^{-1}g = \epsilon(\beta(g))$ and $gg^{-1} = \epsilon(\alpha(g))$.



- An *identity section* $\epsilon : M \to G$ of α and β, such that
  - $\epsilon(\alpha(g))g = g$ and $g\epsilon(\beta(g)) = g$.



A groupoid G over a set M will be denoted simply by the symbol $G \rightrightarrows M$.

The groupoid $G \rightrightarrows M$ is said to be a **Lie groupoid** if G and M are smooth manifolds and all the structural maps are also smooth. In particular α and β are surjective submersions, ϵ is an immersion and ι is a diffeomorphism. Moreover, if $x \in M$, $\alpha^{-1}(x)$ (resp. $\beta^{-1}(x)$) will be called the α-fibre (resp. the β-fibre) of x.

Typical examples of Lie groupoids are: the pair or banal groupoid $M \times M$ over M, a Lie group G (as a Lie groupoid over a single point), the Atiyah groupoid $(M \times M)/G$ (over M/G) associated with a free and proper action of a Lie group G on M, etc.

If $G \rightrightarrows M$ is a Lie groupoid and $g \in G$, then the left-translation by $h \in G$ and the right-translation by h are the diffeomorphisms

$$\begin{aligned} L_h &: \alpha^{-1}(\beta(h)) \to \alpha^{-1}(\alpha(h)), \qquad g \mapsto L_h(g) = hg, \\ R_h &: \beta^{-1}(\alpha(h)) \to \beta^{-1}(\beta(h)), \qquad g \mapsto R_h(g) = gh. \end{aligned}$$

Note that $L_g^{-1} = L_{g^{-1}}$ and $R_g^{-1} = R_{g^{-1}}$.

Similarly to the Lie group case, a vector field $X \in \mathfrak{X}(G)$ is said to be **left-invariant** (resp. **right-invariant**) if it is tangent to the α-fibres (resp. β-fibres) and $X(hg) = T_gL_hX(g)$ (resp. $X(hg) = T_hR_gX(h)$), for $(h, g) \in G_2$.

Lie algebroids

The infinitesimal version of a Lie groupoid is a Lie algebroid, which is defined as follows.

Definition 2.1.6. A **Lie algebroid** is a vector bundle $A \to M$ equipped with a vector bundle morphism $\rho : A \to TQ$ called the **anchor map** and a bracket operation $[\![\cdot, \cdot]\!] : \Gamma(A) \times \Gamma(A) \to \Gamma(A)$ that verifies

$$\begin{aligned} \rho\left([\![X, Y]\!]\right) &= \left[\rho\left(X\right), \rho\left(Y\right)\right], && \text{for } X, Y \in \Gamma(A); \\ [\![X, fY]\!] &= f\,[\![X, Y]\!] + \rho\left(X\right)(f)Y, && \text{for } f \in C^\infty(M, \mathbb{R}). \end{aligned}$$

Given a Lie groupoid $G \rightrightarrows M$, the **associated Lie algebroid** $AG \to M$ is defined by its fibers $A_xG = V_{\epsilon(x)}\alpha = \ker(T_{\epsilon(x)}\alpha)$. There is a bijection between the space $\Gamma(AG)$ and the set of left-invariant vector fields on G. If X is a section of $\tau : AG \to M$, the corresponding left-invariant vector field on G will be denoted $\overleftarrow{X}$ (resp., $\overrightarrow{X}$), where

$$\overleftarrow{X}(g) = T_{\epsilon(\beta(g))}L_g\, X(\beta(g)),$$

for $g \in G$. Using the above facts, one may introduce a bracket $[\![\cdot,\cdot]\!]$ on the space of sections $\Gamma(AG)$ and a bundle map $\rho : AG \to TQ$, which are defined by

$$\overleftarrow{[\![X,Y]\!]} = \left[\overleftarrow{X}, \overleftarrow{Y}\right], \quad \rho(X)(x) = T_{\epsilon(x)}\beta(X(x)),$$

for $X, Y \in \Gamma(AG)$ and $x \in M$.

Using the fact that $[\cdot,\cdot]$ induces a Lie algebra structure on the space of vector fields on G, it is easy to prove that $[\![\cdot,\cdot]\!]$ also defines a Lie algebra structure on $\Gamma(AG)$ verifying the properties of a Lie algebroid bracket.

One can also establish a bijection between sections $X \in \Gamma(AG)$ and right invariant vector fields $\overrightarrow{X} \in \mathfrak{X}(G)$ defined by

$$\overrightarrow{X}(g) = -T_{\epsilon(\alpha(g))}R_g\, T_{\epsilon(\alpha(g))}\iota(X(\alpha(g))),$$

which yields the Lie bracket relation

$$\overrightarrow{[\![X,Y]\!]} = -\left[\overrightarrow{X}, \overrightarrow{Y}\right].$$

2.2 Elements of the calculus of variations

2.2.1 Functionals and their variations

The calculus of variations is based on the concept of a **functional**. A functional is an assignment of a real number to each function (or curve), and it can be regarded as a function whose argument is another function [GF63, chapter 1]. We will be interested in functionals of the form

$$\mathcal{J}[c] = \int_{t_a}^{t_b} L(t, c(t), \dot{c}(t))\mathrm{d}t \tag{2.6}$$

where $c \in \mathcal{F}([t_a, t_b] \subseteq \mathbb{R})$, and $L \in \mathcal{F}'([t_a, t_b] \times \mathbb{R}^n \times \mathbb{R}^n)$, where by $\mathcal{F}$ and $\mathcal{F}'$ we mean two functional spaces.

Although throughout this work we will not need to concern ourselves with complicated function spaces, as we will consider spaces of smooth or at least sufficiently differentiable functions, let us consider here some of the basic spaces that appear frequently in the literature. In particular, let us consider those that appear in [GF63]. These spaces can be summarized as $C^k([t_a, t_b])$ (or $C^k([t_a, t_b], \mathbb{R})$ to be more precise), that is, the space of continuous functions defined on $[t_a, t_b]$ whose derivatives up to and including k are continuous in $[t_a, t_b]$. As it is common elsewhere, we will just write $C^0([t_a, t_b]) \equiv C([t_a, t_b])$. These spaces are considered in conjunction with the norm

$$\|c\|_k = \sum_{i=0}^{k} \max_{t\in I} \left|c^{(i)}(t)\right|$$

where $c^{(0)}$ is understood as c itself. They can be interpreted as the Riemann integral equivalent of the Sobolev spaces $W^{k,\infty}([t_a, t_b])$, that is, spaces of functions whose derivatives up to and including k are in $L^\infty([t_a, t_b])$. It should be noted that we could extend the results in this section to these latter spaces and even bigger by appending the usual *"almost everywhere"* but we will not do this.

A functional $\mathcal{J}$ is said to be continuous at c^* if for any $\epsilon > 0$ there exists a $\delta > 0$ such that $|\mathcal{J}[c] - \mathcal{J}[c^*]| < \epsilon$, with $\|c - c^*\| < \delta$, where $\|\cdot\|$ is the norm of the corresponding function space of choice.

The increment of a functional $\mathcal{J}$ in the *direction* h is defined as

$$\Delta\mathcal{J}_c[h] = \mathcal{J}[c + h] - \mathcal{J}[c],$$

where $h = h(t)$, and the function $c = c(t)$ is fixed.

If we can write the increment as

$$\Delta\mathcal{J}_c[h] = \delta\mathcal{J}_c[h] + \varepsilon \|h\|,$$

where $\delta\mathcal{J}[h]$ is a linear functional and $\varepsilon \to 0$ as $\|h\| \to 0$, then $\mathcal{J}$ is said to be **differentiable** and the linear functional is called a variation of $\mathcal{J}$.

2.2.2 Critical points of a functional and variational problems

In analogy with standard calculus, we say that a differentiable functional $\mathcal{J}$ has a critical point at $c = c^*$ if its variation vanishes at said point, that is, if

$$\delta\mathcal{J}_{c^*}[h] = 0$$

for all admissible h.

The following two lemmas will lay the foundations of the rest of the results that will allow us to characterize such critical points. For their proof and further generalizations, please check [GF63; GH04; Fri10]

Lemma 2.2.1 (**Fundamental lemma of the calculus of variations**). *If* $g(t) \in C([t_a, t_b])$ *and*

$$\int_{t_a}^{t_b} g(t)h(t)\mathrm{d}t = 0$$

for every $h(t) \in C([t_a, t_b])$ *such that* $h(t_a) = h(t_b) = 0$, *then* $g(t) = 0$ *for all* $t \in [t_a, t_b]$.

Lemma 2.2.2 (**Du Bois-Reymond lemma**). *If* $g(t) \in C([t_a, t_b])$ *and*

$$\int_{t_a}^{t_b} g(t)h'(t)\mathrm{d}t = 0 \tag{2.7}$$

for every $h(t) \in C^1([t_a, t_b])$ *such that* $h(t_a) = h(t_b) = 0$, *then* $g(t) = c = const.$ *for all* $t \in [t_a, t_b]$.

The following lemma is also sometimes referred to as the fundamental lemma of the calculus of variations instead of lemma 2.2.1:

Lemma 2.2.3. *If $f(t), g(t) \in C([t_a, t_b])$ and*

$$\int_{t_a}^{t_b} [f(t)h(t) + g(t)h'(t)]\,\mathrm{d}t = 0 \tag{2.8}$$

for every $h(t) \in C^1([t_a, t_b])$ such that $h(t_a) = h(t_b) = 0$, then $g(t) \in C^1([t_a, t_b])$ and $g'(t) = f(t)$ for all $t \in [t_a, t_b]$.

Proof. Let

$$F(t) = \int_{t_a}^{t} f(s)\mathrm{d}s$$

so that if we apply integration by parts on the first term of eq.(2.8), we get

$$\int_{t_a}^{t_b} f(t)h(t)\mathrm{d}t = F(t)h(t)|_{t_a}^{t_b} - \int_{t_a}^{t_b} F(t)h'(t)\mathrm{d}t$$

where the boundary terms vanish due to h vanishing on it. Then we can rewrite (2.8) as

$$\int_{t_a}^{t_b} [-F(t) + g(t)]\,h'(t)\mathrm{d}t = 0$$

Applying now lemma 2.2.2 we know that

$$F(t) - g(t) = \text{const},$$

and thus, by the definition of $F(t)$ we get that

$$g'(t) = f(t)$$

for $t \in [t_a, t_b]$, concluding the proof. □

As we stated in the beginning of this section, the most common type of functional we will deal with is one of the form of eq.(2.6). This is the form of the typical **action functional** that appears in mechanics and the defining function L of the functional is called a Lagrangian.

We can compute the variation of such a functional by using Taylor's theorem on the increment of the functional, that is

$$\begin{aligned}
\Delta\mathcal{J}_c[h] &= \int_{t_a}^{t_b} L(t, c(t) + h(t), \dot{c}(t) + \dot{h}(t))\mathrm{d}t - \int_{t_a}^{t_b} L(t, c(t), \dot{c}(t))\mathrm{d}t \\
&= \int_{t_a}^{t_b} \Big[L(t, c(t) + h(t), \dot{c}(t) + \dot{h}(t)) - L(t, c(t), \dot{c}(t))\Big]\,\mathrm{d}t \\
&= \int_{t_a}^{t_b} [L(t, c(t), \dot{c}(t)) - L(t, c(t), \dot{c}(t))]\,\mathrm{d}t \\
&+ \int_{t_a}^{t_b} \Big[D_2L(t, c(t), \dot{c}(t))h(t) + D_3L(t, c(t), \dot{c}(t))\dot{h}(t)\Big]\,\mathrm{d}t + \epsilon\,\|h\|
\end{aligned}$$

where D_i corresponds to partial differentiation with respect to the i-th argument.

From this we then read,

$$\delta\mathcal{J}_c[h] = \int_{t_a}^{t_b} \Big[D_2L(t, c(t), \dot{c}(t))h(t) + D_3L(t, c(t), \dot{c}(t))\dot{h}(t)\Big]\,\mathrm{d}t$$

A solution $c \in C^1([t_a, t_b])$ of $\delta\mathcal{J}_c[h] = 0$ for all $h \in C^1([t_a, t_b])$ is called a *weak solution of the variational problem* or weak critical point.

Theorem 2.2.4. *Let*

$$\mathcal{J}[c] = \int_{t_a}^{t_b} L(t, c(t), \dot{c}(t))\mathrm{d}t$$

with $c \in C^2([t_a, t_b])$ *weak critical point, that is,*

$$\int_{t_a}^{t_b} \left[D_2L(t, c(t), \dot{c}(t))h(t) + D_3L(t, c(t), \dot{c}(t))\dot{h}(t) \right] \mathrm{d}t = 0$$

for every $h \in C^1([t_a, t_b])$ *with* $h(t_a) = h(t_b) = 0$*, and assume* $D_2L \in C([t_a, t_b])$ *and* $D_3L \in C^1([t_a, t_b])$*. Then* c *satisfies*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(D_3L(t, c(t), \dot{c}(t))\right) - D_2L(t, c(t), \dot{c}(t)) = 0 \tag{2.9}$$

Proof. This theorem can be derived as a direct consequence of lemma 2.2.3. □

The resulting equation, (2.9) is called the **Euler-Lagrange equation**. A solution c satisfying this equation is called a *strong solution of the variational problem*. We will be solely interested in strong solutions throughout this work, and so we will simply call them solutions.

Remark (1). More commonly this theorem can be stated simply for $L \in C^2$, in which case, it suffices to apply integration by parts on the second term of the variations [], namely

$$\int_{t_a}^{t_b} D_3L(t, c(t), \dot{c}(t))\dot{h}(t)\mathrm{d}t = D_3L(t, c(t), \dot{c}(t))h(t)|_{t_a}^{t_b} - \int_{t_a}^{t_b} \frac{\mathrm{d}}{\mathrm{d}t}\left(D_3L(t, c(t), \dot{c}(t))\right) h(t)\mathrm{d}t.$$

Clearly, the boundary term vanishes due to the hypothesis on h and then the same result follows by applying lemma 2.2.1 on the resulting integral. This is by far the most common derivation and one we apply very often in mechanics. △

Remark (2). This theorem gives us a characterization of a critical point of a functional and thus we can say that a necessary condition for $c \in C^k([t_a, t_b])$, with $k \geq 2$, to be a critical point is for it to satisfy the Euler-Lagrange equation.

Note that the Euler-Lagrange equation is of second order, and so its solutions will generally depend on two arbitrary parameters. The most common variational problem is finding a particular curve c satisfying certain admissibility conditions and such that it is a critical point of the functional. These admissibility conditions usually take the form of boundary value conditions, such as

$$c^*(t_a) = c_a, \quad c^*(t_b) = c_b. \qquad \triangle$$

These results can be readily generalized to higher dimensions, that is, for functions $c \in C^2([t_a, t_b], \mathbb{R}^n)$, for $n \in \mathbb{N}$. In this case we would be dealing with $h \in C^1([t_a, t_b], \mathbb{R}^n)$ and each component $h^i(t)$ would be independent of the rest. This leads to Euler-Lagrange equations for each component of c, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{c}^i}(t, c(t), \dot{c}(t))\right) - \frac{\partial L}{\partial c^i}(t, c(t), \dot{c}(t)) = 0, \quad \text{for } i = 1, ..., n$$

where we use the standard notation $\frac{\partial L}{\partial \dot{c}^i}$ instead of something like D_{2_i}.

Note that for each Lagrangian function $L \in C^2$ we get a well-defined set of Euler-Lagrange equations, but it is perfectly possible for two different Lagrangians $L_1, L_2 \in C^2$ to lead to the same set of Euler-Lagrange equations.

Proposition 2.2.1. *Let $c \in C^2([t_a, t_b], \mathbb{R}^n)$ be a critical point of the functional $\mathcal{J}$ defined by the Lagrangian function $L(t, c(t), \dot{c}(t)) \in C^2$. Let also $F = F(t, c(t)) \in C^2$ and define the function*

$$G(t, c(t), \dot{c}(t)) = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial c^i}\dot{c}^i(t).$$

Then c is also a critical point of the functional $\mathcal{J}'$ defined by the Lagrangian $L' = L + G$.

Proof. It suffices to check that for a G so defined, its Euler-Lagrange equations vanish identically, that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial G}{\partial \dot{c}^i}\right) - \frac{\partial G}{\partial c^i} = 0, \quad \text{for } i = 1, ..., n.$$

Then the result follows immediately. □

Remark. This last result can be restated simply as if $L' = L + \frac{\mathrm{d}F}{\mathrm{d}t}$, with $F \in C^2(\mathbb{R} \times \mathbb{R}^n, \mathbb{R})$, and if c is a critical point of L, then c is a critical point of L'. △

2.2.3 Constrained variational problems

We will often find variational problems with further admissibility (also referred to as subsidiary) conditions [see GH04, chapter 2] such as the necessity of $c \in C^k([t_a, t_b], \mathbb{R}^n)$, with $k \geq 2$, to satisfy a certain set of (generally nonlinear) equations

$$\Phi(t, c(t), \dot{c}(t)) = 0, \quad \text{with } \Phi \in C^\ell([t_a, t_b] \times \mathbb{R}^n \times \mathbb{R}^n, \mathbb{R}^m), \ell \geq 1, 1 \geq m \geq n - 1$$

or even inequalities in the context of optimal control (the latter will not be considered here, [see Fri10]). Such equations are called constraints. Obviously, in order for the problem to be well-posed it is necessary for the boundary conditions to be compatible with the constraints.

We will restrict ourselves to constraints of the form

$$\Phi(c(t)) = 0$$

and of the form

$$\Phi(c(t), \dot{c}(t)) = 0$$

The former are called **holonomic** while the latter are frequently called **nonholonomic constraints**. In the context of mechanics, as we will see in chapter 3, we will reserve this latter name precisely for explicitly non-variational problems, whereas variational problems subject to these constraints will be referred to as *variational nonholonomic* or *vakonomic*.

Holonomic constraints can be regarded as a local definition of a manifold M immersed in $\mathbb{R}^n$ with $\dim M = n - m$. We will then refer to M as the **constraint submanifold**. In this setting, c is then a curve which, in order to satisfy the admissibility conditions, must lie on M. Note that this means that in order to generate a variation of c also lying on M, let us call it $\hat{c}$, the generator of such transformation could be interpreted as a vector field tangent to M. Indeed, we can consider a family of curves on $\hat{c}$ on M dependent on some real parameter ϵ such that for $\epsilon = 0$ we get c, so in some local chart we can write

$$c(t, \epsilon) = c(t) + \epsilon h(t) + \mathcal{O}(\epsilon^2).$$

More generally then

$$h = \frac{\mathrm{d}}{\mathrm{d}\epsilon} c_\epsilon \Big|_{\epsilon=0},$$

and thus $h(t) \in T_{c(t)}M$ for every $t \in [t_a, t_b]$ and we can simply write $h \in T_cM$. From the results in the former section we are particularly interested in a certain kind of such vector fields, namely those that vanish at the boundaries t_a and t_b. This leads to the particular definition of the tangent space of a curve satisfying the admissibility conditions as

$$T_cM = \{X : [t_a, t_b] \to TM | \tau_M X = c, X(t_a) = X(t_b) = 0\}$$

We can be more precise and define this with respect to a certain type of curves, $c \in C^k([t_a, t_b], M)$, so that $T_cC^k([t_a, t_b], M)$ is only composed of $C^k([t_a, t_b], TM)$ curves.

If we consider $h \in T_cM$, then the fundamental lemma 2.2.1 implies that, if $g(t)$ is instead considered as an element in the dual of the tangent of c, then $g(t) \in T_c^0M$, where

$$T_c^0M = \{\alpha : [t_a, t_b] \to T^*M | \pi_M \alpha = c, \alpha(X) = 0, \forall X \in T_cM\}$$

is the annihilator of all tangent vectors of c.

In order to compute a variation we can write [see AM78, chapter 2.3.8]

$$\delta\mathcal{J}_c[h] = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{J}[c_\epsilon]\bigg|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\int_{t_a}^{t_b} L(t, c_\epsilon(t), \dot{c}_\epsilon(t))\mathrm{d}t\bigg|_{\epsilon=0}$$

and now $\delta\mathcal{J}_c$ can be interpreted as a differential form acting on the vector h. In that sense we will change our notation slightly and write $\mathrm{d}\mathcal{J}[c](h)$.

Clearly, from this point of view the result of theorem 2.2.4 can also be generalized nicely to the manifold setting where instead of $\mathbb{R}^n$ we deal intrinsically with a smooth manifold N of the same dimension, and the Euler-Lagrange equations are just coordinate expressions of the 1-form $D_{EL}L : \mathbb{R} \times T^{(2)}M \to T^*M$ [see MW01, chapter 1.2]:

$$\int_{t_a}^{t_b} \left\langle D_{EL}L(t, \hat{c}^{(2)}(t)), h(t) \right\rangle \mathrm{d}t = 0$$

If instead we decide to work with M as an immersed manifold in $\mathbb{R}^n$ (or N), then it is possible to modify a given functional to make sure that the first variation is in the annihilator. One just needs to realize two things:

1. the annihilator of T_cM is spanned by $\mathrm{d}\Phi\big|_c$,
2. there must exist functions $\lambda \in C^k([t_a, t_b], \mathbb{R}^m)$, for some $k \geq 0$ such that $D_{EL}L + \lambda \mathrm{d}\Phi\big|_c = 0$.

With this, one can see that if we substitute our Lagrangian function with a modified Lagrangian

$$\tilde{L} = L + \lambda\Phi$$

the corresponding functional $\widetilde{\mathcal{J}}$ will be naturally constrained to M. In fact, if we consider λ to be part of the curve we vary, by theorem 2.2.4, we get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{c}^i}(t, c(t), \dot{c}(t))\right) - \frac{\partial L}{\partial c^i}(t, c(t), \dot{c}(t)) = \lambda^j(t)\frac{\partial \Phi_j}{\partial c^i}(c(t)), \quad & \text{for } i = 1, ..., n, \\ \Phi_j(c(t)) = 0, \quad & \text{for } j = 1, ..., m, \end{aligned}$$

which are necessary conditions for c to be a critical point of the original functional $\mathcal{J}$ simultaneously satisfying the holonomic constraint.

When dealing with variational nonholonomic constraints, the procedure is formally the same as this one, but now the constraint submanifold is a submanifold not of $\mathbb{R}^n$, but of $T\mathbb{R}^n \cong \mathbb{R}^{2n}$. We will not discuss this further but we offer here the necessary conditions for c to be a critical point satisfying the constraints [see Cor+02; BC93; Zam00]:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{c}^i}(t,c(t),\dot{c}(t))\right) - \frac{\partial L}{\partial c^i}(t,c(t),\dot{c}(t)) &= \frac{\mathrm{d}\lambda^j}{\mathrm{d}t}\frac{\partial \Phi_j}{\partial \dot{c}^i}(c(t),\dot{c}(t)) \\ &+ \lambda^j\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \Phi_j}{\partial \dot{c}^i}(c(t),\dot{c}(t))\right) - \frac{\partial \Phi_j}{\partial c^i}(c(t),\dot{c}(t))\right], \quad \text{for } i = 1,...,n, \\ \Phi_j(c(t),\dot{c}(t)) &= 0, \qquad\qquad\qquad\qquad\qquad\qquad \text{for } j = 1,...,m,\end{aligned} \tag{2.10}$$

2.2.4 Total variations

There is a more general type of variation where the evolution parameter t is also a varied function and the boundary values are not fixed [e.g. Fri10, chapter 3.1.2]. The best way to do this is to consider τ as a new unvaried evolution parameter, so that t now depends on τ and ϵ and $t = \tau$ when $\epsilon = 0$, that is,

$$t(\tau,\epsilon) = \tau + \epsilon k(\tau) + \mathcal{O}(\epsilon^2).$$

Geometrically this can be handled in an elegant way using the formalism of jet bundles [see Kra13, for an excellent step-by-step derivation], but this exceeds the scope of what we wish to discuss, so we will limit ourselves to a more analytical formalism.

If we substitute this t in c,

$$c(t(\tau,\epsilon),\epsilon) = q(t(\tau,\epsilon)) + \epsilon h(t(\tau,\epsilon)) + \mathcal{O}(\epsilon^2).$$

where c now varies both on its own and due to the variation of t.

Differentiating with respect to ϵ, we obtain

$$\begin{aligned}K(\tau) &= \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}t(\tau,\epsilon)\right|_{\epsilon=0} = k(\tau) \\ H(\tau) &= \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}c(t(\tau,\epsilon),\epsilon)\right|_{\epsilon=0} = \dot{q}(\tau)k(\tau) + h(\tau) + \mathcal{O}(kh)\end{aligned}$$

We will only consider the case of an unconstrained functional $\mathcal{J}$. The total variation is

$$\Delta\mathcal{J}_c[K,H] = \hat{\delta}\mathcal{J}_c[K,H] + \varepsilon_k \|K\| + \varepsilon_h \|H\|$$

with $\varepsilon_k \to 0$ as $\|K\| \to 0$ and $\varepsilon_h \to 0$ as $\|H\| \to 0$

The variation of the action is

$$\begin{aligned}
\hat{\delta}\mathcal{J}_c[K,H] &= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\int_{t_a=t(\tau_a,\epsilon)}^{t_b=t(\tau_b,\epsilon)} L(t,c(t,\epsilon),\dot{c}(t,\epsilon))\mathrm{d}t\Bigg|_{\epsilon=0} \\
&= \int_{\tau_a}^{\tau_b} \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(L(t(\tau,\epsilon),c(t(\tau,\epsilon),\epsilon),\dot{c}(t(\tau,\epsilon),\epsilon))\frac{\mathrm{d}t}{\mathrm{d}\tau}(\tau,\epsilon)\right)\Bigg|_{\epsilon=0}\mathrm{d}\tau \\
&= \int_{\tau_a}^{\tau_b} \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(L(t(\tau,\epsilon),c(t(\tau,\epsilon),\epsilon),\dot{c}(t(\tau,\epsilon),\epsilon))\right|_{\epsilon=0}\frac{\mathrm{d}t}{\mathrm{d}\tau}(\tau,0)\mathrm{d}\tau \\
&+ \int_{\tau_a}^{\tau_b} L(t(\tau,0),c(t(\tau,0),0),\dot{c}(t(\tau,0),0))\,\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\frac{\mathrm{d}t}{\mathrm{d}\tau}(\tau,\epsilon)\right)\Bigg|_{\epsilon=0}\mathrm{d}\tau \\
&= \int_{\tau_a}^{\tau_b} \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(L(t(\tau,\epsilon),c(t(\tau,\epsilon),\epsilon),\dot{c}(t(\tau,\epsilon),\epsilon))\right|_{\epsilon=0}\mathrm{d}\tau \\
&+ \int_{\tau_a}^{\tau_b} L(\tau,c(\tau),\dot{c}(\tau))\dot{k}(\tau)\mathrm{d}\tau
\end{aligned}$$

The first term gives us

$$\begin{aligned}
&\int_{\tau_a}^{\tau_b}\left[\frac{\partial L}{\partial\tau}(\tau,q(\tau),\dot{q}(\tau))k(\tau) + \frac{\partial L}{\partial c}(\tau,q(\tau),\dot{q}(\tau))\left(\dot{q}(\tau)k(\tau)+h(\tau)\right)\right. \\
&\left.+\,\frac{\partial L}{\partial\dot{c}}(\tau,q(\tau),\dot{q}(\tau))\left(\ddot{q}(\tau)k(\tau)+\dot{h}(\tau)\right)\right]\mathrm{d}\tau \\
&= \int_{\tau_a}^{\tau_b}\left[\left(\frac{\partial L}{\partial\tau}(\tau,q(\tau),\dot{q}(\tau)) + \frac{\partial L}{\partial c}(\tau,q(\tau),\dot{q}(\tau))\dot{q}(\tau) + \frac{\partial L}{\partial\dot{c}}(\tau,q(\tau),\dot{q}(\tau))\ddot{q}(\tau)\right)k(\tau)\right. \\
&\left.+\,\frac{\partial L}{\partial c}(\tau,q(\tau),\dot{q}(\tau))h(\tau) + \frac{\partial L}{\partial\dot{c}}(\tau,q(\tau),\dot{q}(\tau))\dot{h}(\tau)\right]\mathrm{d}\tau \\
&= \int_{\tau_a}^{\tau_b}\left\{\frac{\mathrm{d}}{\mathrm{d}\tau}\left(L(\tau,c(\tau),\dot{c}(\tau))\right)k(\tau)\right. \\
&\left.+\left[\frac{\partial L}{\partial c}(\tau,c(\tau),\dot{c}(\tau)) - \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial L}{\partial\dot{c}}(\tau,c(\tau),\dot{c}(\tau))\right)\right]h(\tau)\right\}\mathrm{d}\tau + \frac{\partial L}{\partial\dot{c}}h(\tau)\Bigg|_{\tau_a}^{\tau_b},
\end{aligned}$$

while the second term gives us, using integration by parts,

$$L(\tau,q(\tau),\dot{q}(\tau))k(\tau)\Big|_{\tau_a}^{\tau_b} - \int_{\tau_a}^{\tau_b}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(L(\tau,c(\tau),\dot{c}(\tau))\right)k(\tau)\mathrm{d}\tau.$$

Putting everything together we see that the total derivatives of L cancel out, leading to

$$\begin{aligned}
&\int_{\tau_a}^{\tau_b}\left[\frac{\partial L}{\partial c}(\tau,c(\tau),\dot{c}(\tau)) - \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial L}{\partial\dot{c}}(\tau,c(\tau),\dot{c}(\tau))\right)\right]h(\tau)\mathrm{d}\tau \\
&+\left[\frac{\partial L}{\partial\dot{c}}(\tau,q(\tau),\dot{q}(\tau))h(\tau) + L(\tau,q(\tau),\dot{q}(\tau))k(\tau)\right]_{\tau_a}^{\tau_b}.
\end{aligned}$$

But $k = K$, and $h = H - \dot{q}K$, and thus we get

$$\int_{\tau_a}^{\tau_b} \left[\frac{\partial L}{\partial c}(\tau, c(\tau), \dot{c}(\tau)) - \frac{\mathrm{d}}{\mathrm{d}\tau} \left(\frac{\partial L}{\partial \dot{c}}(\tau, c(\tau), \dot{c}(\tau)) \right) \right] h(\tau) \mathrm{d}\tau + \frac{\partial L}{\partial \dot{c}}(\tau, q(\tau), \dot{q}(\tau)) H(\tau) \Big|_{\tau_a}^{\tau_b} + \left(L(\tau, q(\tau), \dot{q}(\tau)) - \dot{q}(\tau) \frac{\partial L}{\partial \dot{c}}(\tau, q(\tau), \dot{q}(\tau)) \right) K(\tau) \Big|_{\tau_a}^{\tau_b}.$$

Clearly, if we set $K(\tau_a) = K(\tau_b) = 0$ and $H(\tau_a) = H(\tau_b) = 0$, we get exactly the same result as with a normal variation, but the important terms here are the boundary terms.

2.2.5 Optimal control

An interesting area of application of the theory of calculus of variations other than mechanics is **optimal control** [see Fri10; LVS12; BW99; Blo15]. In chapter 5 we will actually see a case of *optimal control of a mechanical system*, so both fields are not only related but can coalesce.

Control theory is a branch of mathematics that studies the effects of introducing *controls* in a dynamical system. Let a certain system be described by a dynamical system $\dot{y} = f_0(t, y)$, where $y \in \mathbb{R}^n$ and $f_0 \in \mathcal{F}(\mathbb{R} \times \mathbb{R}^n, \mathbb{R}^n)$ are called the *state variables* and the *plant* of the system, and $\mathcal{F}(\mathbb{R} \times \mathbb{R}^n, \mathbb{R}^n)$ is some functional space. Introducing controls in a system usually entails generating a new dynamical system

$$\dot{y} = f(t, y, u)\,,$$

the **control system** (also known as *plant*), such that $f(t, y, 0) = f_0(t, y)$, where the new variables $u \in U$, with $U \subseteq \mathbb{R}^m$ and $0 < m \leq n$, are precisely the *controls*. These allow us to manipulate the original dynamical system influencing its evolution. Control theory is thus a broad subject posing questions such as the feasibility of stirring the system from one state to another given a certain sets of controls (*controllability*), or the generation of control laws that stabilize certain trajectories of the system, among others.

Optimal control is a part of this subject where, given a controllable system and some *optimality criterion*, we are tasked with finding a control law that stirs the system from a given state to another optimally. The optimality criterion is provided by the necessity of extremizing (either minimizing or maximizing) a **cost functional** $\mathcal{J}$. This cost functional is commonly defined by a single **cost function**, $C \in \mathcal{F}'([t_a, t_b] \times \mathbb{R}^n \times \mathbb{R}^m, \mathbb{R})$, although more general terms can appear in the form of **terminal costs**, $\Phi \in \mathcal{F}''([t_a, t_b] \times \mathbb{R}^n)$. Thus, a typical optimal control functional is of the form

$$\mathcal{J}[c] = \Phi(t_b, y(t_b)) + \int_{t_a}^{t_b} C(t, y(t), u(t)) \mathrm{d}t$$

where now $c(t) = (y(t), u(t))$ is a curve in an appropriate space. Although control problems tend to be quite general, needing to take into account the possibility of discontinuous controls and discontinuities in the cost function, among other things, for the purposes of this work we may restrict ourselves to simple C^k spaces with k sufficiently high.

A standard optimal control problem is then a problem of the form

$$\begin{aligned} &\text{Find } (t_b, c) \text{ such that } \min_c \mathcal{J}[c] \\ &\text{subject to:} \\ \dot{y}(t) &= f(t, y(t), u(t)) \\ y(t_a) &= y_a \\ \Psi(t_b, y(t_b)) &= 0 \\ u(t) &\in U, \quad \text{for } t \in [t_a, t_b] \end{aligned} \tag{2.11}$$

where $\Psi(t_b, y(t_b)) \in \mathcal{F}'''([t_a, t_b] \times \mathbb{R}^n, \mathbb{R}^r)$, for $r > 0 \in \mathbb{N}$, is called a **terminal condition**. This formulation already takes into consideration the possibility of not having t_b fixed (optimal time problems). If U had boundaries, then we would need to study the problem of inequality constraints and talk about the Pontryagin maximum (or minimum) principle [see Cla90, chapter 5.2] and the Karush–Kuhn–Tucker (necessary) conditions for optimality [see Fri10, chapter 4.6], which would deviate us too far. Thus, we will assume $U \cong \mathbb{R}^m$.

For such a problem, we can define an extended cost functional including the constraints

$$\begin{aligned} \bar{\mathcal{J}}[\bar{c}] = \Phi(t_b, y(t_b)) &+ \langle \nu, \Psi(t_b, y(t_b)) \rangle \\ &+ \int_{t_a}^{t_b} \left[C(t, y(t), u(t)) + \langle \mu(t), \dot{y}(t) - f(t, y(t), u(t)) \rangle \right] \mathrm{d}t \end{aligned}$$

where $\bar{c}(t) = (y(t), u(t), \mu(t)) \in C^k([t_a, t_b], \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^n)$, and both $\nu \in \mathbb{R}^r$ and $\mu(t) \in \mathbb{R}^n$ are Lagrange multipliers. The latter are called **co-states** in this theory. Let us also define a new function, $L(t, y, \dot{y}, u, \mu) \in C^2$, as the integrand of this functional, and variations

$$\begin{aligned} K(\tau) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} t(\tau, \epsilon)\bigg|_{\epsilon=0} = k(\tau) \\ (H(\tau), V(\tau), \Lambda(\tau)) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} \bar{c}(t(\tau, \epsilon), \epsilon)\bigg|_{\epsilon=0} \\ &= (\dot{y}(\tau)k(\tau) + h(\tau), \dot{u}(\tau)k(\tau) + v(\tau), \dot{\mu}(\tau)k(\tau) + \lambda(\tau)) \end{aligned}$$

such that $K(\tau_a) = 0$, $H(\tau_a) = 0$, $V(\tau_a) = 0$, $\Lambda(\tau_a) = 0$, $t(\tau_a) = t_a$ and $t(\tau_b) = t_b$.

The necessary conditions for optimality are precisely that the *total variations vanish* [see Fri10, chapter 3.3]. Therefore, we can read off from the result of the previous section, with y instead of q, and obtain

$$\begin{aligned} &\int_{\tau_a}^{\tau_b} \left\{ \left[\frac{\partial L}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}\tau} \left(\frac{\partial L}{\partial \dot{y}} \right) \right] h(\tau) + \frac{\partial L}{\partial u} v(\tau) + \frac{\partial L}{\partial \mu} \lambda(\tau) \right\} \mathrm{d}\tau \\ &+ \frac{\partial L}{\partial \dot{y}} H(\tau)\bigg|_{\tau_b} + \left[L - \dot{y} \frac{\partial L}{\partial \dot{y}} \right] K(\tau)\bigg|_{\tau_b}. \end{aligned}$$

We also need to take into account the terms related to the terminal cost and conditions:

$$\left[\frac{\partial \Phi}{\partial t_b} + \left\langle \nu, \frac{\partial \Psi}{\partial t_b} \right\rangle \right] K(\tau_b) + \left[\frac{\partial \Phi}{\partial y(t_b)} + \left\langle \nu, \frac{\partial \Psi}{\partial y(t_b)} \right\rangle \right] H(\tau_b) + \langle \Pi, \Psi(t_b, q(t_b)) \rangle$$

with $\Pi \in \mathbb{R}^r$ arbitrary.

Joining everything together we get the following set of equations after substitution

$$\begin{aligned}
\dot{\mu} &= \frac{\partial C}{\partial y}(t,y,u) - \left\langle \mu, \frac{\partial f}{\partial y}(t,y,u) \right\rangle \\
0 &= \frac{\partial C}{\partial u}(t,y,u) - \left\langle \mu, \frac{\partial f}{\partial u}(t,y,u) \right\rangle \\
\dot{y} &= f(t,y,u) \\
[\langle \mu, \dot{y} \rangle - C(t,y,u)]|_{t=t_b} &= \frac{\partial \Phi}{\partial t_b} + \left\langle \nu, \frac{\partial \Psi}{\partial t_b} \right\rangle \\
\lambda(t_b) &= \frac{\partial \Phi}{\partial y(t_b)} + \left\langle \nu, \frac{\partial \Psi}{\partial y(t_b)} \right\rangle \\
0 &= \Psi(t_b, q(t_b))
\end{aligned}$$

The function $\langle \mu, \dot{y} \rangle - C(t,y,u)$ is usually called the **Hamiltonian** of the optimal control problem.

2.3 Numerical integration

The main reference for this section is [HLW10]. Further references can be found throughout the text for notions not found in those books or not taken from them.

2.3.1 Introduction to the numerical solution of systems of ODEs

Assume we are interested in solving the following generic initial value problem (IVP) numerically:

$$\begin{cases} \dot{y}(t) &= f(t, y(t)) \\ y(t_0) &= y_0 \end{cases} \tag{2.12}$$

where $y(t) \in \mathbb{R}^n$ and $f : I \times \mathbb{R}^n \to T\mathbb{R}^n \cong \mathbb{R}^n$, where $I \subseteq \mathbb{R}$ and $t_0 \in I$, is a sufficiently differentiable time-dependent vector field.

The exact or analytic solution of problem (2.12) is a mapping (a flow) $\Phi : I \times I \times \mathbb{R}^n \to \mathbb{R}^n$, such that $y(t) = y(t_0 + \Delta t) = \Phi_{t_0,\Delta t} y_0, \forall \Delta t \in I$.

A numerical solution of problem (2.12) is a mapping (an approximate flow) $\widetilde{\Phi}_{t_0,h} : y_0 \mapsto y_1$, where $y_1 \approx y(t_0 + h)$. We say the order of approximation of our numerical solution is p if, as $h \to 0$, it satisfies that

$$y_1 - y(t_0 + h) = \mathcal{O}(h^{p+1}),$$

or equivalently,

$$\widetilde{\Phi}_{t_0,h} - \Phi_{t_0,h} = \mathcal{O}(h^{p+1}).$$

We are going to take an interest in methods based on polynomial interpolation rules and more specifically, in collocation type methods. These methods consist of finding a polynomial whose derivative at certain interpolation nodes, known as **collocation points**, coincides with the vector field f of the problem [GS69; Wri92; HNW93].

Continuous collocation

An s-stage continuous collocation polynomial $u(t)$ (of degree s) for problem (2.12) must satisfy:

$$\begin{cases} u(t_0) &= y_0 \\ \dot{u}(t_0 + c_i h) &= f(t_0 + c_i h, u(t_0 + c_i h)), \quad i = 1, ..., s \end{cases}$$

where c_i are distinct real numbers. s is called the *number of stages* of the collocation polynomial. Using Lagrange interpolation the polynomial must be such that:

$$\dot{u}(t) = \sum_{j=1}^{s} k_j \ell_j(t) = \sum_{j=1}^{s} f(t_0 + c_j h, u(t_0 + c_j h))\ell_j(t)$$

where $\ell_j(t)$ is the j-th element of the Lagrange basis of dimension s. Thus, each element of this basis is a polynomial of degree $s - 1$.

The most well-known and widely used methods of this kind are Gauss, Radau and Lobatto methods. We will be focusing on the latter for reasons that will become clear in later chapters.

A Lobatto continuous collocation polynomial has the highest order possible, subject to the condition $c_1 = 0, c_s = 1$, i.e. they must include the endpoints as interpolation nodes. Said interpolation nodes are the zeros of the polynomial $x(x-1)\mathcal{J}_{s-2}^{(1,1)}(2x-1)$, where $\mathcal{J}_n^{(\alpha,\beta)}(x)$ is a Jacobi polynomial. They are also symmetric, meaning $\widetilde{\Phi}_h^{-1} = \widetilde{\Phi}_{-h}$, which warrants that their order is even. Its quadrature order is $p = 2s - 2$, and its lowest order member is the implicit trapezoidal rule.

One of the most salient features of continuous collocation methods is that they provide us with a continuous approximation of the solution between t_0 and $t_1 = t_0 + h$, namely the interpolation polynomial $u(t)$, instead of just a discrete set of points. This polynomial is an approximation of order s to the exact solution [see HLW10, lemma 1.6, p.33], i.e.:

$$\|u(t) - y(t)\| \leq Ch^{s+1} \quad \forall t \in [t_0, t_0 + h] \tag{2.13}$$

and for sufficiently small h.

Moreover, the approximation at quadrature points is of order p (immediate consequence of [HLW10, theorem 1.5, p.32]).

Discontinuous collocation

An s-stage discontinuous collocation polynomial $u(t)$ for problem (2.12) is a polynomial of degree $s - 2$ satisfying:

$$\begin{cases} u(t_0) &= y_0 - hb_1(\dot{u}(t_0) - f(t_0, u(t_0))) \\ \dot{u}(t_0 + c_i h) &= f(t_0 + c_i h, u(t_0 + c_i h)), \quad i = 2, ..., s-1 \\ y_1 &= u(t_1) - hb_s(\dot{u}(t_1) - f(t_0, u(t_1))) \end{cases}$$

where $t_1 = t_0 + h$, b_1, b_s and c_i are distinct real numbers. s is called the *number of stages* of the method. Using Lagrange interpolation the polynomial must be such that:

$$\dot{u}(t) = \sum_{j=2}^{s-1} k_j \ell_{j-1}(t) = \sum_{j=2}^{s-1} f(t_0 + c_j h, u(t_0 + c_j h))\ell_{j-1}(t)$$

where $\ell_j(t)$ is the j-th element of the Lagrange basis of dimension $s-2$. Thus each element of this basis is a polynomial of degree $s - 3$.

Contrary to continuous methods, the generated interpolation polynomial provides a poor continuous approximation of the solution [HLW10, lemma 1.10, p.38], i.e.:

$$\|u(t) - y(t)\| \leq Ch^{s-1} \quad \forall t \in [t_0, t_0 + h], \tag{2.14}$$

and is better seen as providing a scaffolding from which to build an approximation of y_1. Again, we consider Lobatto collocation polynomials, i.e. subject to $c_1 = 0, c_s = 1$. These methods still provide an approximation of order $p = 2s - 2$ for y_1 [HLW10, theorem 1.9, p.37].

Runge-Kutta methods

The collocation methods discussed above can be seen separately as a particular instance of a Runge-Kutta method, completely defined by a set of coefficients (a_{ij}, b_i, c_i), where $\sum_{j=1}^{s} a_{ij} = c_i$. These coefficients are usually arranged in a **Butcher's tableau**,

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

In particular, for continuous collocation methods [GS69; Wri92]:

$$a_{ij} = \int_0^{c_i} \ell_j(\tau)\mathrm{d}\tau, \qquad b_i = \int_0^1 \ell_i(\tau)\mathrm{d}\tau.$$

A numerical solution of (2.12) can be found using an s-stage Runge-Kutta method with coefficients (a_{ij}, b_j, c_i) leading to:

$$\begin{aligned} y_1 &= y_0 + h\textstyle\sum_{j=1}^{s} b_j k_j \\ Y_i &= y_0 + h\textstyle\sum_{j=1}^{s} a_{ij} k_j \\ k_i &= f(t_0 + c_i h, Y_i, Z_i) \end{aligned}$$

In order to analyze the properties of a given Runge-Kutta scheme it is useful to establish a series of *simplifying assumptions* that it satisfies:

$$B(p) : \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k} \quad \text{for } k = 1, ..., p \tag{2.15a}$$

$$C(q) : \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \quad \text{for } i = 1, ..., s,\ k = 1, ..., q \tag{2.15b}$$

$$D(r) : \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = \frac{b_j(1 - c_j^k)}{k} \quad \text{for } j = 1, ..., s,\ k = 1, ..., r \tag{2.15c}$$

When referring to these assumptions for a Runge-Kutta method $(\hat{a}_{ij}, \hat{b}_i)$ we will write them as $\widehat{X}(\hat{y})$.

Lastly, there is a function associated to a Runge-Kutta method that we need to define. Consider the linear problem $\dot{y} = \lambda y$, and apply one step of the given method for an initial value y_0. The function $\mathcal{R}(z)$ defined by $y_1 = \mathcal{R}(h\lambda)y_0$ is the so-called stability function of the method.

For an arbitrary Runge-Kutta method we have that

$$\mathcal{R}(z) = 1 + zb(\mathrm{Id} - zA)^{-1}\mathbb{1},$$

where $A = (a_{ij})$, $b = (b_1, ..., b_s)$ and $\mathbb{1} = (1, ..., 1)^T$. In the particular case of a method satisfying that $a_{sj} = b_j$, which is the case of Lobatto methods, this can be reduced to:

$$\mathcal{R}(z) = e_s(\mathrm{Id} - zA)^{-1}\mathbb{1},$$

where e_i denotes an s dimensional row vector whose entries are all zero except for its i-th entry which is 1.

Partitioned Runge-Kutta methods

Apart from the usual Runge-Kutta methods, there exists a slightly more general class of methods called partitioned Runge-Kutta methods. These methods are of special relevance when the ODE system of problem (2.12) can be partitioned, i.e. it has a natural partition of the form:

$$\begin{cases} \dot{y}(t) &= f(t, y(t), z(t)) \\ \dot{z}(t) &= g(t, y(t), z(t)) \end{cases},$$

where $y(t) \in \mathbb{R}^{n_y}$ and $z(t) \in \mathbb{R}^{n_z}$ with n_y and n_z not necessarily equal.

A particular case is that of problems derived from classical mechanics, where the phase space is usually the cotangent bundle of some manifold Q, T^*Q, which can be partitioned at each point as $Q \times \mathbb{R}^n$ via its local trivialization.

These methods consist of applying different Runge-Kutta schemes to each part in order to take advantage of the structure of the problem. As such, a partitioned Runge-Kutta method is defined by a pair $(a_{ij}, b_i), (\hat{a}_{ij}, \hat{b}_i)$:

$$\begin{array}{llll} y_1 &= y_0 + h\sum_{j=1}^s b_j k_j, & z_1 &= z_0 + h\sum_{j=1}^s \hat{b}_j \ell_j \\ Y_i &= y_0 + h\sum_{j=1}^s a_{ij} k_j, & Z_i &= z_0 + h\sum_{j=1}^s \hat{a}_{ij} \ell_j \\ k_i &= f(t_0 + c_i h, Y_i, Z_i), & \ell_i &= g(t_0 + c_i h, Y_i, Z_i) \end{array}$$

In the realm of time-independent mechanics a very important set of partitioned Runge-Kutta methods arises naturally from the application of the discrete Hamilton's principle (see 3.2.1). These are the so-called symplectic partitioned Runge-Kutta methods, which manage to preserve the symplectic structure of the original problem. Such methods satisfy [HLW10, theorem 4.6, p.193]:

$$\begin{array}{rlrl} b_i\hat{a}_{ij} + \hat{b}_j a_{ji} &= b_i\hat{b}_j, & i, j &= 1, ..., s \\ b_i &= \hat{b}_i, & i &= 1, ..., s \end{array}$$

This means that each of the methods does not need to be symplectic in order for the partitioned method to be overall symplectic.

Note that if (a_{ij}, b_i) and $(\hat{a}_{ij}, \hat{b}_i)$ are two symplectically conjugated methods, each satisfying the symplifying assumptions $B(p), C(q), D(r)$ and $\widehat{B}(\hat{p}), \widehat{C}(\hat{q}), \widehat{D}(\hat{r})$ then $\hat{p} = p$, $C(q)$ implies $\hat{r} = q$, and conversely $D(r)$ implies $\hat{q} = r$.

Apart from these, there are a few more simplifying assumptions that pairs of compatible methods satisfy [see Jay96]:

$$C\widehat{C}(Q): \sum_{j=1}^{s}\sum_{l=1}^{s} a_{ij}\hat{a}_{jl}c_l^{k-2} = \frac{c_i^k}{k(k-1)} \quad \text{for } i=1,...,s,\ k=2,...,Q$$

$$D\widehat{D}(R): \sum_{i=1}^{s}\sum_{j=1}^{s} b_i c_i^{k-2} a_{ij}\hat{a}_{jl} = \frac{b_l}{k(k-1)}\left[(k-1)-(kc_l-c_l^k)\right] \quad \text{for } l=1,...,s,\ k=2,...,R$$

$$\widehat{C}C(\hat{Q}): \sum_{j=1}^{s}\sum_{l=1}^{s} \hat{a}_{ij}a_{jl}c_l^{k-2} = \frac{c_i^k}{k(k-1)} \quad \text{for } i=1,...,s,\ k=2,...,\hat{Q}$$

$$\widehat{D}D(\hat{R}): \sum_{i=1}^{s}\sum_{j=1}^{s} \hat{b}_i c_i^{k-2} \hat{a}_{ij}a_{jl} = \frac{\hat{b}_l}{k(k-1)}\left[(k-1)-(kc_l-c_l^k)\right] \quad \text{for } l=1,...,s,\ k=2,...,\hat{R}$$

It can be shown that if both methods are symplectically conjugated, then $Q = R = p-r$ and $\hat{Q} = \hat{R} = p-q$. In particular, Lobatto III A and B methods, which will be very important for us, satisfy $B(2s-2)$, $C(s)$, $D(s-2)$, $\widehat{B}(2s-2)$, $\widehat{C}(s-2)$, $\widehat{D}(s)$, as well as $C\widehat{C}(s), D\widehat{D}(s), \widehat{C}C(s-2), \widehat{D}D(s-2)$ respectively.

2.3.2 Momentum and symplecticity conservation

A non-constant function $I(y)$ is a **first integral** of eq.(2.12) if

$$\frac{\mathrm{d}}{\mathrm{d}t}I(y) = I'(y)f(y) = 0, \quad \forall y.$$

In mechanics these are referred to as *conserved quantities* or *constants of the motion*. Some of the more well-known ones in that context are *linear momentum* (linear first integrals), *angular momentum* and the symplectic form (both of which classify as mixed quadratic (2.16)), and *energy* (generally fully nonlinear).

Methods preserving the latter will not be the focus of this work and instead we will focus on methods preserving the other quantities. Still, some very interesting results that will appear later (see 3.2.4) will show us that the methods considered will have very good energy behavior.

Theorem 2.3.1 (**Conservation of linear first integrals**). *[HLW10, theorem IV.1.5, pg.99] Every Runge-Kutta method conserves linear first integrals. Partitioned Runge-Kutta methods also conserve linear first integrals if $b_i = \hat{b}_i$ or if the first integral only depends on either y or z.*

Proof. The proof for Runge-Kutta methods can be found in [HLW10]. The proof for partitioned Runge-Kutta methods can be done similarly: Let $I(y,z) = L_y y + L_z z$, with L_y, L_z constant functions, then $L_y f(y,z) + L_z g(y,z) = 0$ for all y and z. In particular,

for partitioned RK methods it must be true that $L_y k_i + L_z \ell_i = 0$, for $i = 1, ..., s$. Then,

$$\begin{aligned} I(y_1, z_1) &= L_y y_1 + L_z z_1 \\ &= L_y \left(y_0 + h \sum_{j=1}^{s} b_j k_j \right) + L_z \left(z_0 + h \sum_{j=1}^{s} \hat{b}_j \ell_j \right) \\ &= L_y y_0 + L_z z_0 + h \sum_{j=1}^{s} b_j L_y k_j + h \sum_{j=1}^{s} \hat{b}_j L_z \ell_j \\ &= I(y_0, z_0) + h \sum_{j=1}^{s} \left(b_j L_y k_j + \hat{b}_j L_z \ell_j \right) \end{aligned}$$

Thus, in order to have conservation the second term must vanish, which leads us to the result of the theorem. □

Arbitrary quadratic forms are not generally conserved for all RK. Only symplectic methods, such as Gauss methods, conserve these. The situation is even worse for partitioned RK methods, for which this is impossible. Nevertheless, there is a subset of quadratic forms, let us call them *mixed*, of the form

$$I(y, z) = y^T L z \tag{2.16}$$

with $L \in M_{n_y, n_z}(\mathbb{R})$ that some partitioned RK methods can preserve.

Theorem 2.3.2 (**Conservation of mixed quadratic first integrals**). *[HLW10, theorem IV.2.4, pg.103] Consider a partitioned RK method with coefficients* (a_{ij}, b_j), $(\hat{a}_{ij}, \hat{b}_j)$. *If the coefficients satisfy*

$$\begin{aligned} &b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j, \quad \text{for } i, j = 1, ..., s \\ &b_i b_j = b_j \end{aligned}$$

then it conserves mixed first integral of the form (2.16).

The proof is similar to the proof of the theorem above but it now involves the equations for the stages. This conservation is particularly important in mechanics, as stated above, because this implies the conservation of the canonical symplectic form, hence the added adjective *symplectic* for the partitioned methods that satisfy the hypotheses of the theorem.

2.3.3 Order conditions

Order conditions for a Runge-Kutta type method are derived by comparing the Taylor series of the exact solution of (2.12) with the solution obtained via our numerical method. This spans a very rich theory developed by Butcher and others during the second half of last century, using tools such as rooted trees, Hopf algebras and group theory. We will not be delving into the latter two.

Focusing on the autonomous case, the idea is to consider the exact solution $y(t), t \in [t_0, t_0 + h]$ of:

$$\begin{cases} \dot{y}(t) &= f(y(t)) \\ y(t_0) &= y_0 \end{cases} \tag{2.17}$$

Our main goal is to compute the Taylor expansion of $y(t_0 + h)$ in powers of h and compare same order terms. We can compute higher derivatives by inserting our solution in f and recursively using the chain rule as:

$$\begin{aligned}
\dot{y} &= f(y) \\
\ddot{y} &= f'(y)\dot{y} \\
y^{(3)} &= f''(y)(\dot{y},\dot{y}) + f'(y)\ddot{y} \\
y^{(4)} &= f^{(3)}(y)(\dot{y},\dot{y},\dot{y}) + 3f''(y)(\ddot{y},\dot{y}) + f'(y)y^{(3)} \\
&\vdots
\end{aligned}$$

after which we eliminate all derivatives from the right-hand side, starting from the top, by inserting the preceding formulas:

$$\dot{y} = f \tag{2.18a}$$
$$\ddot{y} = f'f \tag{2.18b}$$
$$y^{(3)} = f''(f,f) + f'f'f \tag{2.18c}$$
$$y^{(4)} = f'''(f,f,f) + 3f''(f'f,f) + f'f''(f,f) + f'f'f'f \tag{2.18d}$$
$$\vdots$$

Each term on the right-hand side has a diagrammatic representation in terms of **rooted-trees**, and each successive differentiation can be easily obtained by grafting new branches onto each node (or *vertex*) of the tree.

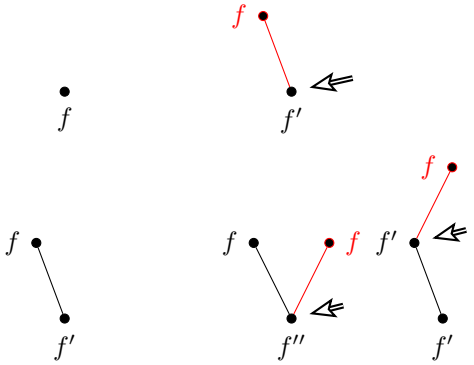


Figure 2.1: The first line shows how to go from eq.(2.18a) to eq.(2.18b), and the second how to go from eq.(2.18b) to eq.(2.18c). Taking the bottom right trees, we can see that if we were to continue expanding from them, there would be three terms with the exact same configuration corresponding to the term $f''(f'f,f)$: two coming from the tree on the left and one coming from the tree on the right. This leads to the factor 3 multiplying that term in eq.(2.18d)

Definition 2.3.1. The set of **rooted trees** $\mathfrak{T}$ is recursively defined as follows:

1. The graph $\bullet$ with only one node, called the root, is in $\mathfrak{T}$.
2. If $\tau_1, ..., \tau_k \in \mathfrak{T}$, the graph obtained by grafting their respective roots to a new node (see fig.2.2) also belongs to $\mathfrak{T}$. This is denoted by

$$\tau = [\tau_1, ..., \tau_k],$$

and the new node is the root of τ. The relative ordering of the different $\tau_i \in \mathfrak{T}$ is irrelevant.

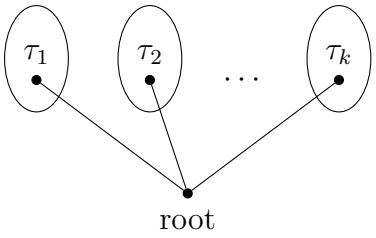
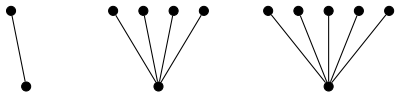


Figure 2.2: Rooted tree construction by grafting existing trees to new root

Trees $\tau = [\bullet, ..., \bullet]$ are called **bushy trees**, as graphically they are dense and short (see fig. 2.3).

Figure 2.3: Sample bushy trees of orders 2, 5 and 6 respectively



The order (or degree) of the tree, $|\tau|$, coincides with the number of nodes contained in τ. Let us denote by $F : \mathfrak{T} \times \mathbb{R}^n \to \mathbb{R}^n$ the map defined recursively by $F_\bullet(y) = f(y)$ and

$$F_\tau(y) = f^{(k)}(y)\left(F_{\tau_1}(y), ..., F_{\tau_k}(y)\right), \quad \text{for } \tau = [\tau_1, ..., \tau_k].$$

Each instance of this is called an **elementary differential**. If we collect all combinatorial coefficients that appeared in the expansion, most of which were 1 except for the 3 in eq.(2.18d), in a symbol α_τ, then we may write the q-th derivative of y compactly as:

$$y^{(q)}(t_0) = \sum_{|\tau|=q} \alpha_\tau F_\tau(y_0) \tag{2.19}$$

Now, let us move on to our numerical methods, which are of the form

$$g_i = hf(u_i),$$

$$u_i = y_0 + \sum_j a_{ij} g_j, \quad y_1 = y_0 + \sum_j b_j g_j.$$

Considering g_i, u_1 and y_1 as functions of h we can expand the former in terms of h. Based on

$$g_i^{(q)} = \left(h\tilde{f}(h)\right)^{(q)} = h\tilde{f}^{(q)}(h) + q\tilde{f}^{(q-1)}(h),$$

where $\tilde{f}(h) = f(u_i(h))$, we see that when $h = 0$ we get

$$g_i^{(q)} = q\left(f(u_i)\right)^{(q-1)}.$$

If we expand this, we get essentially the same as with the exact solution except for the factor q.

$$\begin{aligned}
\dot{g}_i &= 1 \cdot (f(y_0)) \\
\ddot{g}_i &= 2 \cdot (f'(y_0)\dot{u}_i) \\
g_i^{(3)} &= 3 \cdot (f''(y_0)(\dot{u}_i, \dot{u}_i) + f'(y_0)\ddot{u}_i) \\
g_i^{(4)} &= 4 \cdot (f'''(y_0)(\dot{u}_i, \dot{u}_i, \dot{u}_i) + 3f''(y_0)(\ddot{u}_i, \dot{u}_i) + f'(y_0)u_i^{(3)}) \\
&\vdots
\end{aligned}$$

Using the derivatives of $u_i^{(q)} = \sum_j a_{ij} g_j^{(q)}$ and successively substituting derivatives in the right-hand side again, we are left with expressions:

$$\begin{aligned}
\dot{g}_i &= 1 \cdot (f) \\
\ddot{g}_i &= 2 \cdot \left(\sum_j a_{ij} f' f \right) \\
g_i^{(3)} &= 3 \cdot \left(\sum_{jk} a_{ij} a_{ik} f''(f, f) \right) + (2 \cdot 3) \cdot \left(\sum_{jk} a_{ij} a_{jk} f' f' f \right) \\
g_i^{(4)} &= 4 \cdot \left(\sum_{jk\ell} a_{ij} a_{ik} a_{i\ell} f'''(f, f, f) \right) + (2 \cdot 4) \cdot \left(3 \cdot \sum_{jk\ell} a_{ij} a_{jk} a_{i\ell} f''(f' f, f) \right) \\
&\quad + (3 \cdot 4) \cdot \left(\sum_{jk\ell} a_{ij} a_{jk} a_{j\ell} f' f''(f, f) \right) + (2 \cdot 3 \cdot 4) \cdot \left(\sum_{jk\ell} a_{ij} a_{jk} a_{k\ell} f' f' f' f \right) \\
&\quad \vdots
\end{aligned}$$

Again this leads to compact expressions:

$$u_i^{(q)}(t_0) = \sum_{|\tau|=q} \gamma_\tau \, \varepsilon_{i,\tau} \, \alpha_\tau F_\tau(y_0) \tag{2.20}$$

$$g_i^{(q)}(t_0) = \sum_{|\tau|=q} \gamma_\tau \, \delta_{i,\tau} \, \alpha_\tau F_\tau(y_0) \tag{2.21}$$

where the new factors $\varepsilon_{i,\tau}, \delta_{i,\tau}$ are the factors containing terms in a_{ij}, and $\gamma(\tau)$ are the integer coefficients appearing in each term that do not belong in α_τ. For $\tau = [\tau_1, ..., \tau_k]$ we have that

$$\begin{aligned}
\varepsilon_{i,\tau} &= \sum_j a_{ij} \delta_{j,\tau} \\
\delta_{i,\tau} &= \varepsilon_{i,\tau_1} \cdot ... \cdot \varepsilon_{i,\tau_k}, \\
\gamma_\tau &= |\tau| \, \gamma_{\tau_1} \cdot ... \cdot \gamma_{\tau_k},
\end{aligned}$$

Finally, using the notation:

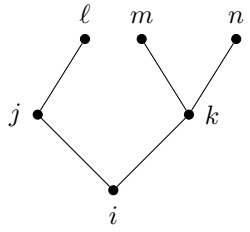
$$\phi_\tau = \sum_i b_i \delta_{i,\tau}$$

the derivatives of the numerical solution at $h = 0$ become:

$$y_1^{(q)} = \sum_{|\tau|=q} \gamma_\tau \phi_\tau \alpha_\tau F_\tau(y_0) \tag{2.22}$$

Comparing eqs.(2.19) and (2.22) we get that the corresponding method will be of order p iff [HLW10, theorem III.1.5, p.56]:

$$\phi_\tau = \frac{1}{\gamma_\tau} \quad \text{for } |\tau| \leq p. \tag{2.23}$$



Example 2.3.1. Let us denote the order 6 tree represented on the left by τ. It can be schematically written as $\tau = [\tau_1, \tau_2] = [[\bullet], [\bullet, \bullet]]$. The ϕ coefficient associated with this tree is

$$\begin{aligned}\phi_\tau &= \sum_{i,j,k,\ell,m,n} b_i a_{ij} a_{j\ell} a_{ik} a_{km} a_{kn} \\ &= \sum_{i,j,k} b_i a_{ij} c_j a_{ik} c_k^2\end{aligned}$$

while, if $\gamma_{\tau_1} = 2$ and $\gamma_{\tau_2} = 3$, the γ coefficient is

$$\gamma_\tau = |\tau| \gamma_{\tau_1} \gamma_{\tau_2} = 6 \cdot 2 \cdot 3 = 36\,,$$

and thus $\phi_\tau = 1/36$.

The same can be done for the inner stages of a method. It is easy to see that if we consider $y(t) = y(t_0 + ch), c \in [0, 1]$, then (2.19) becomes:

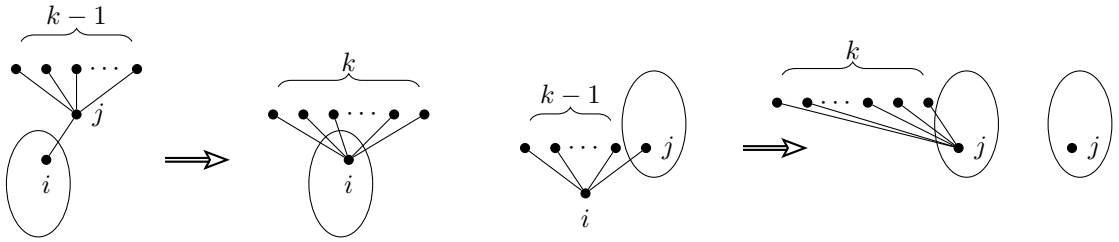
$$y_i^{(q)}(t_0) = c_i^q \sum_{|\tau|=q} \alpha_\tau F_\tau(y_0) \tag{2.24}$$

Proposition 2.3.1. *The order of approximation of the i-th stage, y_i, of a method will be k iff:*

$$\varepsilon_{i,\tau} = \frac{c_i^k}{\gamma_\tau}, \quad \textit{for } |\tau| \leq k; \tag{2.25}$$

Proof. Direct comparison of each order in (2.24) and (2.20) shows sufficiency. As in [HLW10, theorem III.1.5, p.56], necessity comes from independence of each $F(\tau)$. □

These results ((2.23) and (2.25)) are intimately related to the so-called simplifying assumptions (2.15). One can use the latter to perform what is commonly referred to as tree reduction, which serves to reduce the height of the tree, turning it bushier instead.



(a) Reduction using C (2.15b). (b) Reduction using D (2.15c).

Figure 2.4: Tree height reduction using simplifying assumptions (2.15).

Order conditions for partitioned methods

Let us consider the following IVP for an autonomous partitioned system

$$\begin{cases} \dot{y}(t) &= f(y(t), z(t)) \\ \dot{z}(t) &= g(y(t), z(t)) \\ y(t_0) &= y_0 \\ z(t_0) &= z_0 \end{cases} \tag{2.26}$$

Similarly to the non-partitioned case we may expand the exact solution around t_0:

$$\begin{aligned}
\dot{y} &= f(y,z) \\
\ddot{y} &= f_y(y,z)\dot{y} + f_z(y,z)\dot{z} \\
y^{(3)} &= f_{yy}(y,z)(\dot{y},\dot{y}) + 2f_{y,z}(y,z)(\dot{y},\dot{z}) + f_{z,z}(y,z)(\dot{z},\dot{z}) + f_y(y,z)\ddot{y} + f_z(y,z)\ddot{z} \\
&\vdots \\
\dot{z} &= g(y,z) \\
\ddot{z} &= g_y(y,z)\dot{y} + g_z(y,z)\dot{z} \\
z^{(3)} &= g_{yy}(y,z)(\dot{y},\dot{y}) + 2g_{y,z}(y,z)(\dot{y},\dot{z}) + g_{z,z}(y,z)(\dot{z},\dot{z}) + g_y(y,z)\ddot{y} + g_z(y,z)\ddot{z} \\
&\vdots
\end{aligned}$$

and eliminate the derivatives of y and z from the right-hand side.

$$\begin{aligned}
\dot{y} &= f \\
\ddot{y} &= f_y f + f_z g \\
y^{(3)} &= f_{yy}(f,f) + 2f_{y,z}(f,g) + f_{z,z}(g,g) + f_y f_y f + f_y f_z g + f_z g_y f + f_z g_z g \\
&\vdots \\
\dot{z} &= g \\
\ddot{z} &= g_y f + g_z g \\
z^{(3)} &= g_{yy}(f,f) + 2g_{y,z}(f,g) + g_{z,z}(g,g) + g_y f_y f + g_y f_z g + g_z g_y f + g_z g_z g \\
&\vdots
\end{aligned}$$

Once more we can rewrite these equations more compactly by using trees, but we need a more general set of these.

Definition 2.3.2. The set of **rooted bi-colored trees** $\mathfrak{T}^2$ is recursively defined as follows:

1. $\bullet, \circ \in \mathfrak{T}^2$.
2. If $\tau_1, ..., \tau_k \in \mathfrak{T}^2$, the graph obtained by grafting their respective roots onto a new node, $\bullet$ or $\circ$, also belongs to $\mathfrak{T}^2$. This is denoted respectively by
$$\tau = [\tau_1, ..., \tau_k]_\bullet, \quad \tau = [\tau_1, ..., \tau_k]_\circ$$
and the new node is the root of τ. The relative ordering of the different $\tau_i \in \mathfrak{T}^2$ is irrelevant.

We will use the notation $\mathfrak{T}^2_\bullet, \mathfrak{T}^2_\circ \subset \mathfrak{T}^2$ for the sets of trees whose roots are $\bullet$ or $\circ$ respectively. Using bi-colored trees we can then use $\bullet$ to represent a term in f and $\circ$ to represent a term in g (or y and z respectively). Thus, we may write:

$$y^{(q)}(t_0) = \sum_{|\tau_\bullet|=q} \alpha_{\tau_\bullet} F_{\tau_\bullet}(y_0, z_0), \quad \text{for } \tau_\bullet \in \mathfrak{T}^2_\bullet, \tag{2.27a}$$

$$z^{(q)}(t_0) = \sum_{|\tau_\circ|=q} \alpha_{\tau_\circ} F_{\tau_\circ}(y_0, z_0), \quad \text{for } \tau_\circ \in \mathfrak{T}^2_\circ. \tag{2.27b}$$

The same can be done with the numerical solution, where now we just need to redefine

$$\varepsilon_{i,\tau_\bullet} = \sum_j a_{ij}\delta_{j,\tau_\bullet} \quad \phi_{\tau_\bullet} = \sum_i b_i \delta_{i,\tau_\bullet}$$
$$\varepsilon_{i,\tau_\circ} = \sum_j \hat{a}_{ij}\delta_{j,\tau_\circ} \quad \phi_{\tau_\circ} = \sum_i \hat{b}_i \delta_{i,\tau_\circ}$$

for $\tau_\bullet \in \mathfrak{T}^2_\bullet$ and $\tau_\circ \in \mathfrak{T}^2_\circ$. This way, for $h = 0$, we can write

$$y_1^{(q)} = \sum_{|\tau_\bullet|=q} \gamma_{\tau_\bullet}\phi_{\tau_\bullet}\alpha_{\tau_\bullet}F_{\tau_\bullet}(y_0, z_0), \quad \text{for } \tau_\bullet \in \mathfrak{T}^2_\bullet,$$
$$z_1^{(q)} = \sum_{|\tau_\circ|=q} \gamma_{\tau_\circ}\phi_{\tau_\circ}\alpha_{\tau_\circ}F_{\tau_\circ}(y_0, z_0), \quad \text{for } \tau_\circ \in \mathfrak{T}^2_\circ,$$

and the order condition that must be satisfied is exactly eq.(2.23) for each variable.

2.3.4 Backward error analysis

Another powerful tool in the analysis of numerical methods is that of *backward error analysis*. This is in opposition to the analysis we have shown up until now, which could be classified as *forward error analysis*, where we study the error of the numerical method with respect to the solution. In backward error analysis one looks for a modified differential equation, $\dot{\tilde{y}} = \tilde{f}(\tilde{y}, h)$, which our numerical method solves exactly and compares with the original one. It is assumed that the modified equation can be written as a series of the form

$$\dot{\tilde{y}} = \tilde{f}_1(\tilde{y}) + h\tilde{f}_2(\tilde{y}) + h^2\tilde{f}_3(\tilde{y}) + ...$$

where $\tilde{f}_1 = f$ is the original vector field and $\tilde{f}_i$, with $i \geq 2$, can be constructed from an expansion in terms of f and its derivatives.

If we also assume that the discrete flow generated by our numerical method can be expanded as

$$\tilde{\Phi}_h(\tilde{y}) = \tilde{y} + hf(\tilde{y}) + h^2 d_2(\tilde{y}) + h^3 d_3(\tilde{y}) + ...$$

then we can reconstruct the modified equation by comparing terms of the same order up to a certain order p. One of the first results of the theory is the following [HLW10, theorem XI.1.2, pg. 340]

Theorem 2.3.3. *Suppose that the method $y_{n+1} = \tilde{\Phi}_h(y_n)$ is of order p, i.e.,*

$$\tilde{\Phi}_h(y) = \Phi_h(y) + h^{p+1}\delta_{p+1}(y) + \mathcal{O}(h^{p+2}),$$

where $\Phi_t(y)$ denotes the exact flow of $\dot{y} = f(y)$, and $h^{p+1}\delta_{p+1}(y)$ the leading term of the local truncation error. The modified equation then satisfies

$$\dot{\tilde{y}} = f(\tilde{y}) + h^p f_{p+1}(\tilde{y}) + ..., \quad \tilde{y}(0) = y_0,$$

with $f_{p+1}(y) = \delta_{p+1}(y)$.

Another interesting theorem shows why symmetric methods can show better results than expected in some cases [HLW10, theorem XI.2.2, pg. 342]

Theorem 2.3.4. *The coefficients functions of the modified equation of a symmetric method satisfy $f_j(y) = 0$ for even j, consequently the expansion of the modified equation only contains even powers of h.*

By far the most powerful and important results for us are those involving symplectic methods, but we will state them in section 3.2.4 after we have introduced the concept of a Hamiltonian and its importance in mechanics.

2.3.5 Constrained systems and differential-algebraic equations.

Part of the work of this thesis (see chapter 5) is devoted to the numerical solution of mechanical systems with constraints. Such systems lead to IVP of a more general form than that of eq.(2.12). This new type of systems involve not only differential equations but also algebraic equations, and this is the reason why they receive the name of differential-algebraic equations (DAEs) [HLR89]. The generic form of these systems is

$$F(Y, \dot{Y}) = 0, \quad \text{with } F : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m$$

but this is far too general for the scope of this work.

There are several classifications of systems of this type. A simple classification is based on the **differential index** of the system defined as the minimum integer k such that the system

$$\begin{aligned} F(Y, \dot{Y}) &= 0, \\ \frac{\mathrm{d}}{\mathrm{d}t} F(Y, \dot{Y}) &= 0, \\ &\vdots \\ \frac{\mathrm{d}^k}{\mathrm{d}t^k} F(Y, \dot{Y}) &= 0, \end{aligned}$$

can be solved for $\dot{Y}$ in terms of Y, i.e. $\dot{Y} = \dot{Y}(Y)$ [see HLR89; GLG85].

The canonical example of a system of index 1 is one of the form

$$\begin{cases} \dot{y}(t) &= f(y(t), z(t)) \\ 0 &= g(y(t), z(t)) \end{cases}$$

such that $(g_z)^{-1}$ exists around the solution. In this case we have that $Y = (y(t), z(t))$ and derivation of the second equation leads to

$$g_y(y(t), z(t))\dot{y}(t) + g_z(y(t), z(t))\dot{z}(t) = 0$$

Thus, upon substitution of the first equation in this one, we get

$$\begin{cases} \dot{y}(t) &= f(y(t), z(t)) \\ \dot{z}(t) &= -\left(g_z\right)^{-1}(y(t), z(t)) \left[g_y(y(t), z(t)) f(y(t), z(t))\right] \end{cases}$$

The canonical example of a system of index 2 is

$$\begin{cases} \dot{y}(t) &= f(y(t), z(t)) \\ 0 &= g(y(t)) \end{cases} \tag{2.28}$$

such that $(g_y f_z)^{-1}$ exists around the solution. Mechanical systems with nonholonomic constraints fall in this category.

Differentiating the second equation we get

$$g_y(y(t))\dot{y}(t) = g_y(y(t))f(y(t), z(t)) = 0,$$

and a second differentiation leads us to

$$g_{yy}(f, f) + g_y f_z f + g_y f_z \dot{z} = 0.$$

This way we can write

$$\begin{cases} \dot{y} &= f \\ \dot{z} &= -\left(g_y f_z\right)^{-1} \left[g_{yy}(f, f) + g_y f_z f\right] \end{cases}$$

The canonical example of a system of index 3 is

$$\begin{cases} \dot{y}(t) &= f(y(t), z(t)) \\ \dot{z}(t) &= g(y(t), z(t), w(t)) \\ 0 &= k(y(t)) \end{cases}$$

such that $(k_y f_z g_w)^{-1}$ exists around the solution. Mechanical systems with holonomic constraints fall in this category.

In order to solve numerically the IVP associated with a DAE one can apply the same theory as for ordinary differential equations, but the analysis required to prove convergence becomes much more involved. In chapter 5 we will perform a new analysis for a subset of DAE problems of index 2, namely partitioned index 2 problems of the form

$$\begin{cases} \dot{y}(t) &= f(y(t), z(t)) \\ \dot{z}(t) &= g(y(t), z(t), w(t)) \\ 0 &= k(y(t), z(t)) \end{cases} \tag{2.29}$$

such that $(k_z g_w)^{-1}$ exists around the solution. The form of these systems is reminiscent of that of systems of index 3, and it is precisely the sort of system that appears in nonholonomic mechanical systems.

In [HLR89] the authors study systems of index 2 of the type (2.28). In that case bi-colored trees can be applied but the meaning of the nodes $\circ$ differs from what we have seen here and not all tree variations appear in the expansion. Furthermore, they require their methods to be such that the matrix $A = (a_{ij})$ is invertible. In [Jay93] the author studies the case where A is not invertible but a submatrix of it, $\widetilde{A} = (a_{ij})_{i,j\geq 2}$, is. This is the case of Lobatto IIIA methods.

We will perform a similar analysis for systems of type (2.29) using partitioned methods satisfying certain conditions, focusing on symplectic pairs of Lobatto IIIA-B methods, which are the ones that arise naturally as variational integrators in unconstrained systems. Unfortunately, the analysis is even more complex as we need to deal with the multiple interactions of $A = (a_{ij})$, $\widehat{A} = (\hat{a}_{ij})$ and the inverse of $\widetilde{A} = (a_{ij})_{i,j\geq 2}$, leading to the necessity of analyzing which terms can actually appear in the expansion of the system and the use of tri-colored trees.

2.3.6 Numerical integration on Lie groups

We will briefly discuss a particular technique to numerically solve IVP on Lie groups. Let us begin with a general ODE on the Lie group G.

$$\dot{g}(t) = \Phi(t, g(t))$$

This can be recast into a form which will be easier to work with:

$$\dot{g}(t) = T_e L_{g(t)} \phi(t, g(t)) \equiv g(t)\phi(t, g(t))$$

where $\phi : I \times G \to \mathfrak{g}$, with $I = [t_0, t_0 + h]$. An IVP would be one where we are given $g(t_0) = g_0 \in G$.

There are several known ways to numerically solve these problems on Lie groups such as projection methods, Crouch-Grossman methods and Runge-Kutta-Munthe-Kaas [see HLW10; Mun99]. We will focus on the latter, and in particular we will offer a derivation of the resulting continuous collocation methods here.

The idea of these methods is, again, to generate a continuous approximation to a solution curve g, but now this curve must lie on the Lie group G. As we are no longer working on a simple vector space, operations such as addition and translation of vectors in different tangent spaces or the generation of tangent vectors from two points must be carefully reconsidered. To sidestep this problem, we can try to move to a common linear space, such is the case of the Lie algebra $\mathfrak{g}$.

Retractions and their trivialized tangents

Consider a retraction on G which we will write as $\tau : \mathfrak{g} \to \mathbb{R}$. This may be the natural exponential map on G or any other retraction such as the **Cayley map** (or Cayley transform), $\mathrm{cay} : \mathfrak{g} \to G$,

$$\mathrm{cay}(\xi) = (I + \xi/2)^{-1} (I - \xi/2), \quad \xi \in \mathfrak{g},$$

which is available to us for so-called *quadratic* matrix Lie groups such as $SO(n)$ and $SE(n)$.

We should mention here, as it will be necessary in what follows, that given a retraction τ with tangent map $T\tau : T\mathfrak{g} \to TG$, we can define the so-called left and right-trivialized tangents $\mathrm{d}^L\tau, \mathrm{d}^R\tau : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ as the maps defined by [Ise+00a; BM09]

$$\begin{aligned}(T_\xi \tau)\eta &= T_e L_{\tau(\xi)} \left(\mathrm{d}^L\tau_\xi \eta\right), \quad \eta \in T_\xi\mathfrak{g} \cong \mathfrak{g} \\ (T_\xi \tau)\eta &= T_e R_{\tau(\xi)} \left(\mathrm{d}^R\tau_\xi \eta\right).\end{aligned}$$

Note that it is a linear map in its second argument and it can be interpreted as a translation transformation such that if $\eta \in T_\xi\mathfrak{g}$, then its transported image on $T_0\mathfrak{g}$ is either $\mathrm{d}^L\tau_\xi\eta$ or $\mathrm{d}^R\tau_\xi\eta$.

For matrix Lie groups, we have the following formulas to compute the trivialized tangents of the exponential map [Ise+00b]:

$$\mathrm{d}^L \exp_\xi = \sum_{j=0}^{\infty} \frac{(-1)^j}{(j+1)!} \mathrm{ad}_\xi^j, \qquad \mathrm{d}^R \exp_\xi = \sum_{j=0}^{\infty} \frac{1}{(j+1)!} \mathrm{ad}_\xi^j. \tag{2.30}$$

We will generally work with the left trivialization but similar results will hold using the right trivialization. We can in fact relate both as follows. First,

$$\begin{aligned} T_eL_{\tau(\xi)}\left(\mathrm{d}^L\tau_\xi\eta\right) &= T_eR_{\tau(\xi)}\left(\mathrm{d}^R\tau_\xi\eta\right), \\ \Rightarrow \left(\mathrm{d}^L\tau_\xi\eta\right) &= \left(T_eL_{\tau(\xi)}\right)^{-1}T_eR_{\tau(\xi)}\left(\mathrm{d}^R\tau_\xi\eta\right), \\ &= T_{\tau(\xi)}L_{\tau(-\xi)}T_eR_{\tau(\xi)}\left(\mathrm{d}^R\tau_\xi\eta\right), \\ &= \mathrm{Ad}_{\tau(-\xi)}\left(\mathrm{d}^R\tau_\xi\eta\right). \end{aligned}$$

Now consider the following lemma:

Lemma 2.3.5. *[BM09, lemma 4.3] Let $\mathrm{d}^L\tau, \mathrm{d}^R\tau : \mathfrak{g}\times\mathfrak{g} \to \mathfrak{g}$ be the left and right-trivialized tangents to a retraction $\tau : \mathfrak{g} \to G$ respectively, and $\mathrm{Ad}_g : \mathfrak{g} \to \mathfrak{g}$ the adjoint operation of an element $g \in G$. Then the following relations hold:*

$$\begin{aligned} \mathrm{d}^L\tau_\xi &= \mathrm{Ad}_{\tau(-\xi)}\mathrm{d}^L\tau_{-\xi} \\ \mathrm{d}^R\tau_\xi &= \mathrm{Ad}_{\tau(\xi)}\mathrm{d}^R\tau_{-\xi} \end{aligned}$$

Proof. From the identity $\tau(\xi)\tau(-\xi) = e$, by direct differentiation we find that:

$$T_{\tau(\xi)}R_{\tau(-\xi)}T_\xi\tau = -T_{\tau(-\xi)}L_{\tau(\xi)}T_{-\xi}\tau.$$

Now,

$$\begin{aligned} T_{-\xi}\tau &= -\left(T_{\tau(-\xi)}L_{\tau(\xi)}\right)^{-1}T_{\tau(\xi)}R_{\tau(-\xi)}T_\xi\tau \\ &= -T_eL_{\tau(-\xi)}T_{\tau(\xi)}R_{\tau(-\xi)}T_\xi\tau, \end{aligned}$$

and using the chain rule, $\left(T_{-\xi}\tau\right)\eta = -T_eR_{\tau(-\xi)}\left(\mathrm{d}^R\tau_{-\xi}\eta\right)$. Inserting this in the last equation we find that

$$\begin{aligned} -T_eR_{\tau(-\xi)}\mathrm{d}^R\tau_{-\xi} &= -T_eL_{\tau(-\xi)}T_{\tau(\xi)}R_{\tau(-\xi)}T_eR_{\tau(\xi)}\mathrm{d}^R\tau_\xi \\ T_eR_{\tau(-\xi)}\mathrm{d}^R\tau_{-\xi} &= T_eL_{\tau(-\xi)}\mathrm{d}^R\tau_\xi \\ \mathrm{d}^R\tau_{-\xi} &= (T_eR_{\tau(-\xi)})^{-1}T_eL_{\tau(-\xi)}\mathrm{d}^R\tau_\xi \\ &= T_{\tau(-\xi)}R_{\tau(\xi)}T_eL_{\tau(-\xi)}\mathrm{d}^R\tau_\xi \\ &= \mathrm{Ad}_{\tau(-\xi)}\mathrm{d}^R\tau_\xi \end{aligned}$$

from which we can read the result for the right-trivialized tangent after moving the adjoint operator to the left hand side of the equation. The result for $\mathrm{d}^L\tau_\xi$ can be obtained similarly. □

Using the result of lemma 2.3.5 we immediately arrive at

$$\mathrm{d}^L\tau_\xi = \mathrm{d}^R\tau_{-\xi}.$$

We may also define the inverse trivialized tangent as the algebraic inverse of each of these trivialized tangents, $\left(\mathrm{d}^L\tau_\xi\right)^{-1}$ and $\left(\mathrm{d}^R\tau_\xi\right)^{-1}$. Geometrically this can be defined in a similar manner to what we did for the direct tangents: let $(g, v) \in TU_e \subseteq TG$, where $U_e \subseteq G$ is a neighborhood of the identity where the inverse of τ is well defined. The inverse map $T\tau^{-1}$ maps elements in TU_e to elements in $T\mathfrak{g} \cong \mathfrak{g}\times\mathfrak{g}$. Thus $\mathrm{d}^L\tau^{-1}, \mathrm{d}^R\tau^{-1} : \mathfrak{g}\times\mathfrak{g} \to \mathfrak{g}$ must be such that:

$$\left(T_g\tau^{-1}\right)v = \mathrm{d}^L\tau_\xi^{-1}\left(T_gL_{g^{-1}}v\right) = \mathrm{d}^R\tau_\xi^{-1}\left(T_gR_{g^{-1}}v\right)$$

Continuous collocation on a Lie group

As we wish to generate a *collocation* approximation of $g(t)$, which we will call $u(t)$, it must satisfy:

$$\begin{cases} u(t_0) &= g_0 \\ \dot{u}(t_0 + c_i h) &= u(t_0 + c_i h)\phi(t_0 + c_i h, u(t_0 + c_i h)), \quad \forall i = 1, ..., s \end{cases}$$

where $c_i \in \mathbb{R}$ are the collocation coefficients of the s-stage (continuous) collocation method.

Equipped with a retraction, and owing to the linear structure of the Lie algebra, we can generate a polynomial approximant in $\mathfrak{g}$,

$$\xi(t) = \sum_j^s \eta^j \int_0^t \ell_j(\sigma)\mathrm{d}\sigma,$$

with $\ell_i(\sigma)$ being the i-th element of the s-dimensional Lagrange basis associated with the c_i coefficients and $\eta^i \in T_{\xi(t)}\mathfrak{g} \cong \mathfrak{g}$ being fixed elements which can be chosen.

Similar to what we would do in the vector space case we can start with an ansatz of the form:

$$u(t_0 + \lambda h) = g_0\tau(h\xi(\lambda)) = g_0\tau\left(h\sum_j^s \eta^j \int_0^\lambda \ell_j(\sigma)\mathrm{d}\sigma\right)$$

This clearly satisfies the first condition that our collocation approximant must satisfy.

Now we need to impose the second condition to determine the η's. Using $L_j(\lambda) = \int_0^\lambda \ell_j(\sigma)\mathrm{d}\sigma$, we get:

$$\begin{aligned} \dot{u}(t_0 + \lambda h) &= g_0 T\tau\left(h\sum_j^s \eta^j L_j(\lambda)\right)\left(\sum_j^s \eta^j \ell_j(\lambda)\right) \\ &= g_0\tau\left(h\sum_j^s \eta^j L_j(\lambda)\right)\mathrm{d}^L\tau_{h\sum_j^s \eta^j L_j(\lambda)}\left(\sum_j^s \eta^j \ell_j(\lambda)\right) \\ &= u(t_0 + \lambda h)\mathrm{d}^L\tau_{h\sum_j^s \eta^j L_j(\lambda)}\left(\sum_j^s \eta^j \ell_j(\lambda)\right), \end{aligned}$$

thus:

$$\mathrm{d}^L\tau_{h\sum_j^s \eta^j L_j(c_i)}\left(\sum_j^s \eta^j \ell_j(c_i)\right) = \phi\left(t_0 + c_i h, g_0\tau\left(h\sum_j^s \eta^j L_j(c_i)\right)\right). \tag{2.31}$$

From [GS69] we have the following relations between Runge-Kutta coefficients and collocation polynomials:

$$a_{ij} = L_j(c_i) \qquad b_j = L_j(1)$$

We also know that $\ell_j(c_i) = \delta_{ij}$, so we can finally express eq.(2.31) as:

$$\mathrm{d}^L\tau_{h\sum_j^s a_{ij}\eta^j}\eta^i = \phi\left(t_0 + c_i h, g_0\tau\left(h\sum_j^s a_{ij}\eta^j\right)\right). \tag{2.32}$$

For its application to variational integrators we are interested in the case where $\phi(t, g(t))$ is the (left-)trivialised velocity of the system. If we introduce some auxiliary variables ξ^i to simplify the expressions, we finally obtain:

$$\begin{aligned} \xi^i &= h \sum_{j=1}^{s} a_{ij} \eta^j, \\ G^i &= g_0 \tau(\xi^i), \\ \left(G^i\right)^{-1} V^i &= \mathrm{d}^L \tau_{\xi^i} \eta^i, \\ g_1 &= g_0 \tau \left(h \sum_{j=1}^{s} b_j \eta^j \right). \end{aligned}$$

Chapter 3

Geometric description of mechanical systems

3.1 Lagrangian and Hamiltonian mechanics

3.1.1 Lagrangian description

The Lagrangian description of a mechanical system starts with a choice of the space where the system is going to evolve. We will assume it is an n-dimensional smooth manifold Q, which will receive the name of **configuration manifold**. Let also TQ denote its tangent bundle with canonical projection $\tau_Q : TQ \to Q$. If we consider local coordinates (q^i) on Q, $i = 1, ..., n$ and corresponding adapted coordinates on TQ, (q^i, v^i), then, consequently $\tau_Q(q^i, v^i) = (q^i)$. In this context, TQ is commonly called *velocity phase space*.

Next, we need a function that encodes the information of the system. This will be a C^2 function $L : TQ \to \mathbb{R}$. We call such a function the **Lagrangian** of the system. The pair (Q, L) constitutes a **Lagrangian system** [AM78].

In principle the Lagrangian could also depend on a parameter $t \in \mathbb{R}$ called *time*, rendering it a function $L : \mathbb{R} \times TQ \to \mathbb{R}$. These Lagrangians are called time-dependent, for obvious reasons, but will not be considered here.

For simple mechanical systems the Lagrangian can be decomposed into two main terms, $L = T - V$ where

$$T(q, v) = \sum_{i,j=1}^{n} \frac{1}{2} g(q)_{ij} v^i v^j,$$

with $g \in \mathcal{T}_2^0(Q)$, a positive-definite symmetric (i.e. $g(q)_{ij} = g(q)_{ji}$) tensor field, which in Riemannian geometry is called a metric tensor. This term receives the name of *kinetic energy* of the system. The term V is called a *potential* and it frequently depends only on q. If in a chart T only depends on v, that is, $T(v^1, ..., v^n) - V(q^1, ..., q^n)$, the system is called *separable*. This will not play an important role for the development of this work, but it is included here for the sake of completeness.

Let us now consider curves $c : [t_a, t_b] \subseteq \mathbb{R} \to Q$ of class C^2 connecting two fixed points $q_a, q_b \in Q$. Let us denote the collection of all these curves as

$$C^2(q_a, q_b, [t_a, t_b]) = \left\{ c : [t_a, t_b] \to Q \,|\, c \in C^2([t_a, t_b]), c(t_a) = q_a, c(t_b) = q_b \right\}.$$

and its tangent space as

$$T_c C^2(q_a, q_b, [t_a, t_b]) = \\ \left\{ X : [t_a, t_b] \to TQ \,|\, X \in C^1([t_a, t_b]), \tau_Q \circ X = c \text{ and } X(t_a) = X(t_b) = 0 \right\}.$$

Given a Lagrangian L we define its *action functional* as

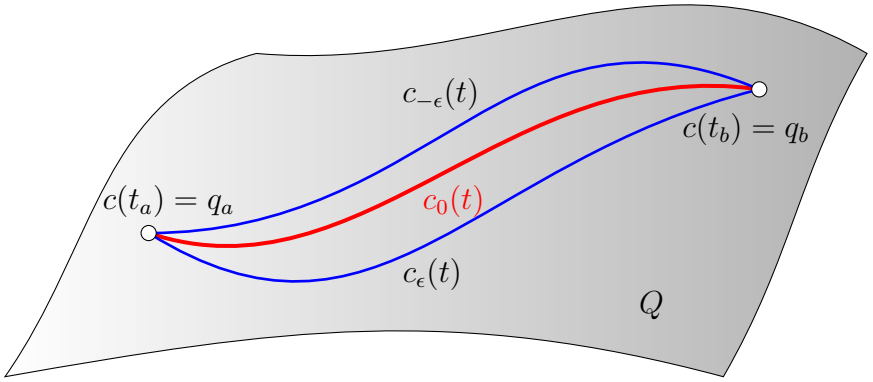
$$\begin{aligned} \mathcal{J} : \quad C^2(q_a, q_b, [t_a, t_b]) &\to \mathbb{R} \\ c &\mapsto \int_{t_a}^{t_b} L(\hat{c}(t))\mathrm{d}t \end{aligned}$$

where $\hat{c}(t) = (c(t), \dot{c}(t))$ is the tangent lift of the curve c.

The main principle that relates the Lagrangian and its action to the motion of the mechanical system can be summarized as follows.

Definition 3.1.1. (Hamilton's principle). A curve $c \in C^2(q_a, q_b, [t_a, t_b])$ is the *physical trajectory* of the Lagrangian system defined by $L : TQ \to \mathbb{R}$ if and only if c is a critical point of the functional $\mathcal{J}$, i.e. $\mathrm{d}\mathcal{J}[c](\delta c) = 0$, for all $\delta c \in T_c C^2(q_a, q_b, [t_a, t_b])$.

In these terms, physical trajectory means that the physical system after which our Lagrangian system is modeled will describe the same motion as predicted from said solution. This principle is also called the *principle of stationary action*.



Using the standard techniques from variational calculus (see theorem 2.2.4), we can show that the curves $c(t) = (q^i(t))$, solutions of the Lagrangian system defined by L, are the solutions of the following system of second order implicit differential equations:

$$D_{\mathrm{EL}} L(\hat{c}^{(2)}) = \left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} \right) \mathrm{d}q^i = 0$$

which are the well-known Euler-Lagrange equations describing the motion of the system. Note that $D_{\mathrm{EL}} L$ can be regarded as a map $D_{\mathrm{EL}} L : T^{(2)}Q \to T^*Q$ over Q, where $T^{(2)}Q \subset TTQ$ is the second order tangent bundle of Q (see section 2.1.2).

Let us denote by $X_L : TQ \to TTQ$ the SODE vector field implicitly defined by the Euler-Lagrange equations, and abusing the notation, let us also use this to refer to its restriction to $T^{(2)}Q$, then we can write

$$D_{\mathrm{EL}} L \circ X_L = 0$$

Poincaré-Cartan forms and energy

As we are working on a tangent bundle TQ, we have at our disposal all the tools we have seen in section 2.1.2, such as the canonical endomorphism $S = \mathrm{d}q^i \otimes \frac{\partial}{\partial v^i}$ and the Liouville vector field $\triangle = v^i \frac{\partial}{\partial v^i}$. Using these tools we can generate important objects in the geometric description of Lagrangian mechanics.

The **Poincaré-Cartan 1 and 2-forms** are defined by $\theta_L = S^*(\mathrm{d}L)$ and $\omega_L = -\mathrm{d}\theta_L$, where S^* denotes the adjoint operator of S [see LR89; Fec06]. In local coordinates these read as

$$\begin{aligned}\theta_L &= \frac{\partial L}{\partial v^i}\,\mathrm{d}q^i,\\ \omega_L &= \mathrm{d}q^i \wedge \mathrm{d}\left(\frac{\partial L}{\partial v^i}\right).\end{aligned}$$

Interestingly, if we remove the constraint $\delta c(t_a) = \delta c(t_b) = 0$ in Hamilton's principle, then what we obtain after variation is:

$$\mathrm{d}\mathcal{J}[c](\delta c) = \int_{t_a}^{t_b} \left\langle D_{EL}L(\hat{c}^{(2)}(t)), \delta c(t)\right\rangle \mathrm{d}t + \frac{\partial L}{\partial \dot{q}^i}(q(t),\dot{q}(t))\delta q^i(t)\Big|_{t_a}^{t_b}$$

where $\delta c(t) = (\delta q^i(t))$. As we see, the boundary terms can be rewritten as

$$\langle \theta_L(\hat{c}(t)), \delta c(t)\rangle|_{t_a}^{t_b}\ .$$

This gives us a purely variational way to obtain the Poincaré-Cartan 1-form, and it also has an important consequence. If we denote by $F_L^{\Delta t} : TQ \to TQ$ the flow generated by the Euler-Lagrange vector field X_L with $\Delta t = t_b - t_a$, then, if c is a solution of the Euler-Lagrange equations defined in $[t_a, t_b]$, we can write

$$\mathrm{d}\mathcal{J}[c] = \left(\left(F_L^{\Delta t}\right)^* \theta_L - \theta_L\right)(\hat{c}(t_a))$$

Furthermore, as we know that $\mathrm{d}^2 = 0$, then

$$\mathrm{d}^2\mathcal{J}[c] = 0 \Leftrightarrow \left(F_L^{\Delta t}\right)^* \omega_L = \omega_L$$

which means that the flow preserves the Poincaré-Cartan 2-form.

We can also generate an important function called the **energy** of the system as $E_L = \triangle(L) - L$, with coordinate expression

$$E_L(q,v) = v^i \frac{\partial L}{\partial v^i} - L(q,v).$$

This quantity is preserved for time-independent Lagrangian systems. To see this, one can multiply the Euler-Lagrange equations by $\dot{q}^i$ and then manipulate the expression

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right)\dot{q}^i - \frac{\partial L}{\partial q^i}\dot{q}^i &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i\right) - \frac{\partial L}{\partial q^i}\dot{q}^i - \frac{\partial L}{\partial \dot{q}^i}\ddot{q}^i\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i - L\right)\\ &= \frac{\mathrm{d}}{\mathrm{d}t}E_L(q,\dot{q})\\ &= 0\end{aligned}$$

If we compute a total variation of the action functional as in section 2.2.4, and evaluate along a solution of the Euler-Lagrange equation c, we can identify the extra term that appears beside the Poincaré-Cartan 1-form as $-E_L$:

$$\begin{aligned} \mathrm{d}\mathcal{J}[c] &= \theta_L(\hat{c}(t_b)) - \theta_L(\hat{c}(t_a)) - (E_L(\hat{c}(t_b))\mathrm{d}t_b - E_L(\hat{c}(t_a))\mathrm{d}t_a) \\ &= \left(\left(F_L^{\Delta t}\right)^* \theta_L - \theta_L\right)(\hat{c}(t_a)) - \left(\left(F_L^{\Delta t}\right)^* E_L \mathrm{d}t - E_L \mathrm{d}t\right)(\hat{c}(t_a)) \end{aligned} \tag{3.1}$$

so now we can interpret this as a form on the extended space $\mathbb{R} \times TQ$.

Fibre derivative and symplecticity

We may construct the transformation $\mathbb{F}L : TQ \to T^*Q$, called **fibre derivative** (or *Legendre transform*), defined by

$$\langle \mathbb{F}L(v_q), w_q \rangle = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} L(v_q + t w_q),$$

where $v_q, w_q \in TQ$. In coordinates, this takes the form

$$\mathbb{F}L(q, v) = \left(q^i, \frac{\partial L}{\partial v^i}(q, v)\right)$$

We say that the Lagrangian is regular if $\mathbb{F}L$ is a local diffeomorphism, which in local coordinates is equivalent to the regularity of the Hessian matrix whose entries are

$$(g_L)_{ij} = \frac{\partial^2 L}{\partial v^i \partial v^j}. \tag{3.2}$$

Note that if the Lagrangian is of the simple mechanical form shown above, then g_L coincides with the metric tensor g, and thus it is always regular.

If L is regular, then ω_L is a non-degenerate exact form and so it is a symplectic form on TQ. As the flow of the Euler-Lagrange equations is a (local) diffeomorphism and preserves ω_L, it is said to be a (local) **symplectomorphism**.

Observe that in this case, the Euler-Lagrange equations can be written as a system of explicit second order differential equations, that is, of the form

$$\ddot{q}^i = F^i(q, \dot{q}).$$

The Euler-Lagrange equations can also be geometrically encoded as the equations for the flow of the Hamiltonian vector field $X_{E_L} \equiv X_L$:

$$\imath_{X_L} \omega_L = \mathrm{d}E_L,$$

which allows us to prove energy conservation in another way:

$$\mathcal{L}_{X_L} E_L = \imath_{X_L} \mathrm{d}E_L = \imath_{X_L} \imath_{X_L} \omega_L = 0,$$

where Cartan's magic formula has been used in the first step and the antisymmetry of ω_L has been used in the last step.

Given any pair of vector fields, $V, W \in \mathfrak{X}(TQ)$, it can be shown after some tedious computations involving Cartan's magic formula, eq.(2.3) and (2.4) that

$$\imath_W \imath_{S(V)} \omega_L = -\imath_{S(W)} \imath_V \omega_L \,.$$

If we consider the relation [see LR89, proposition 7.13, pg. 303]

$$\imath_{\triangle}\omega_L = -S^*(\mathrm{d}E_L)\,,$$

this implies that, for any $Y \in \mathfrak{X}(TQ)$,

$$\begin{aligned}\imath_Y\imath_{\triangle}\omega_L &= -\imath_Y S^*(\mathrm{d}E_L)\\ &= -\imath_{S(Y)}\mathrm{d}E_L\\ &= -\imath_{S(Y)}\imath_{X_L}\omega_L\\ &= \imath_Y\imath_{S(X_L)}\omega_L\end{aligned}$$

and therefore if ω_L is symplectic, the Euler-Lagrange vector field must indeed be a SODE (see section 2.1.2) as stated above, that is,

$$S(X_L) = \triangle\,.$$

Interestingly, the Euler-Lagrange equations can be equivalently encoded as [see JS98, chapter 3.4.2]

$$\mathcal{L}_{X_L}\theta_L = \mathrm{d}L, \tag{3.3}$$

which can be easily shown by either carrying out coordinate computations or using Cartan's magic formula again and the definitions of E_L and θ_L.

One final way to express the Euler-Lagrange equations is in conjunction with a vector field on Q. Let $V \in \mathfrak{X}(Q)$, then the Euler-Lagrange vector field satisfies [see Fec06, chapter 18]

$$X_L(V^vL) - V^cL = 0\,. \tag{3.4}$$

which can be easily checked using coordinate computations.

Noether's theorem

Let G be a Lie group with Lie algebra $\mathfrak{g}$ and let it act on Q with the action $\phi : G\times Q \to Q$, $(g,q) \mapsto \phi(g,q)$. Consider the tangent lift of this action, $\hat{\phi} : G \times TQ \to TQ$, $(g, v_q) \mapsto \hat{\phi}(g, v_q) \equiv (T\phi_g)v_q$, where in local coordinates we have

$$\hat{\phi}(g, v_q) = \left(\phi^i(g,q), \frac{\partial\phi^i}{\partial q^j}(g,q)v^j\right).$$

Consider now the integral curve $g : \mathbb{R} \to G$, with $g(0) = e$, generated by the Lie algebra element $\xi \in \mathfrak{g}$, that is, $\dot{g}(0) = \xi$. We say that $\xi_Q \in \mathfrak{X}(Q)$, defined by

$$\xi_Q(q) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\phi(g(t),q)\right|_{t=0},$$

is the **infinitesimal generator** of the action $\phi_{g(t)}$, and similarly $\xi_{TQ} = \xi^c_Q \in \mathfrak{X}(TQ)$,

$$\xi_{TQ}(v_q) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\hat{\phi}(g(t),v_q)\right|_{t=0},$$

is the infinitesimal generator of $\hat{\phi}_{g(t)}$. In local coordinates these take the form

$$\begin{aligned}\xi_Q(q) &= \left(q^i, \frac{\partial\phi^i}{\partial g^k}(e,q)\xi^k\right)\\ \xi_{TQ}(v_q) &= \left(q^i, v^i, \frac{\partial\phi^i}{\partial g^k}(e,q)\xi^k, \frac{\partial^2\phi^i}{\partial g^k\partial q^j}(e,q)\xi^k v^j\right)\end{aligned}$$

Theorem 3.1.1 (**Noether's theorem**). *[e.g. MW01] Let (Q, L) be a Lagrangian mechanical system and assume that L is invariant under the lifted action $\hat{\phi}$ for a curve $g(t)$ generated by $\xi \in \mathfrak{g}$, that is,*

$$L \circ \hat{\phi}_{g(t)} = L, \quad \forall t\,.$$

Then

$$\langle \theta_L, \xi_{TQ} \rangle = \frac{\partial L}{\partial \dot{q}^i} \xi_Q^i$$

is a conserved quantity.

Proof. One way to see this is as follows: Assume c is a physical solution, i.e.

$$\mathrm{d}\mathcal{J}[c](X) = 0,$$

for all $X \in T_c C^2(q_a, q_b, [0, T])$. In particular, we can choose X such that $X(t) = \xi_Q(c(t))$, so the varied paths can be interpreted as generated by $c_\epsilon(t) = \phi\left(\exp(\epsilon\xi), c(t)\right)$, where $\exp(\epsilon\xi) = g(\epsilon)$. This in turn means that for this particular choice

$$\begin{aligned}
\mathrm{d}\mathcal{J}[c](X) &= \int_0^T \frac{\mathrm{d}}{\mathrm{d}\epsilon} L(\hat{c}_\epsilon(t))\bigg|_{\epsilon=0} \mathrm{d}t \\
&= \int_0^T \xi_{TQ}\left(L(\hat{c}(t))\right) \mathrm{d}t \\
&= 0.
\end{aligned}$$

But this then implies that

$$\langle \theta_L(\hat{c}(t)), \xi_{TQ}(\hat{c}(t)) \rangle \big|_0^T = 0$$

which is precisely what we set to prove.

A different way to prove this is by taking eq.(3.4), and taking $V = \xi_Q$. Then, as $\xi_Q^c(L) = \xi_{TQ}(L) = 0$, the equation reduces to

$$X_L(\xi_Q^v(L)) = 0\,.$$

Noting that

$$\begin{aligned}
\langle \theta_L, \xi_{TQ} \rangle &= \langle S^*(\mathrm{d}L), \xi_{TQ} \rangle \\
&= \langle \mathrm{d}L, S(\xi_{TQ}) \rangle \\
&= \left\langle \mathrm{d}L, \xi_Q^v \right\rangle \\
&= \xi_Q^v(L)
\end{aligned}$$

where we have used eq.(2.1.2), then

$$X_L(\langle \theta_L, \xi_{TQ} \rangle) = 0\,.$$

□

If we define the **Lagrangian momentum map**, $J_L : TQ \to \mathfrak{g}^*$ by the relation

$$\langle J_L(v_q), \xi \rangle_{\mathfrak{g}} = \langle \theta_L, \xi_{TQ} \rangle = \imath_{\xi_{TQ}} \theta_L,$$

then we say that under the conditions of Noether's theorem the momentum map is conserved along the flow.

If a momentum map is such that the following diagram commutes, then it is said to be **equivariant**

$$\begin{array}{ccc} TQ & \xrightarrow{\mathcal{J}_L} & \mathfrak{g}^* \\ {\scriptstyle \hat{\phi}_g}\downarrow & & \downarrow{\scriptstyle \mathrm{Ad}^*_{g^{-1}}} \\ TQ & \xrightarrow{\mathcal{J}_L} & \mathfrak{g}^* \end{array}$$

Every Lagrangian momentum map for a G-invariant Lagrangian L is equivariant, as can be shown from the fact that then $\hat{\phi}_* \theta_L = \theta_L$.

3.1.2 Hamiltonian description

The Hamiltonian description of mechanics takes place in the cotangent bundle of the configuration manifold Q. As we have seen in section 2.1.2, T^*Q is equipped with a canonical and exact symplectic structure $\omega_Q = -\mathrm{d}\theta_Q$, where θ_Q is the canonical 1-form on T^*Q. In canonical (adapted) coordinates these become

$$\begin{aligned} \theta_Q &= p_i \mathrm{d}q^i \,, \\ \omega_Q &= \mathrm{d}q^i \wedge \mathrm{d}p_i \,. \end{aligned}$$

Given a Hamiltonian function $H : T^*Q \to \mathbb{R}$ in C^1 we can define its Hamiltonian vector field by

$$\imath_{X_H} \omega_Q = \mathrm{d}H$$

which can be written locally as

$$X_H = \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i}.$$

Its integral curves are determined by **Hamilton's equations**,

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i}(q,p) \,, \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i}(q,p) \,. \end{aligned}$$

Clearly, these equations induce a symplectic flow $F_H^{\Delta t} : T^*Q \to T^*Q$, the **Hamiltonian flow**, as they derive from a Hamiltonian vector field, which is automatically a symplectic vector field. In the language of classical mechanics we say that any diffeomorphism on T^*Q that respects the symplectic form (i.e. a symplectomorphism) is a **canonical transformation**. This means that Hamiltonian flow can be regarded itself as a canonical transformation.

We know that ω_Q induces a Poisson bracket on T^*Q, which allows us to write these equations locally as

$$\begin{aligned} \dot{q}^i &= \left\{ q^i, H \right\} , \\ \dot{p}_i &= \left\{ p_i, H \right\} . \end{aligned}$$

It is easy to see using the antisymmetry of the Poisson bracket that H is a conserved quantity of the flow,

$$\dot{H} = \{H, H\} = 0.$$

Given a Hamiltonian function, H, we may construct a Hamiltonian analogue of the fibre derivative in Lagrangian mechanics, that is, the transformation $\mathbb{F}H : T^*Q \to TQ$ defined by

$$\langle \beta_q, \mathbb{F}H(\alpha_q)\rangle = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} H(\alpha_q + t\beta_q),$$

where $\alpha_q, \beta_q \in T^*Q$. In adapted local coordinates, this takes the form

$$\mathbb{F}H(q,p) = \left(q^i, \frac{\partial H}{\partial p_i}(q,p)\right).$$

We say that a Hamiltonian is regular if its fibre derivative $\mathbb{F}H$ is a local diffeomorphism, which in local coordinates is equivalent to the regularity of the Hessian matrix whose entries are:

$$(g_H)^{ij} = \frac{\partial^2 H}{\partial p_i \partial p_j}. \tag{3.5}$$

If we have a regular Lagrangian mechanical system (Q, L), we can define an associated Hamiltonian function as $H = E_L \circ (\mathbb{F}L)^{-1}$. Additionally, one gets that $\theta_L = (\mathbb{F}L)^* \theta_Q$ and $\omega_L = (\mathbb{F}L)^* \omega_Q$, which proves once again if L is regular, then ω_L provides TQ with a symplectic structure. In this particular case, $\mathbb{F}H = \mathbb{F}L^{-1}$ and we also get that $\mathbb{F}L_* X_{E_L} = X_H$.

Momentum map

As in the Lagrangian setting, let G be a Lie group with Lie algebra $\mathfrak{g}$ and let it act on Q with the action $\phi : G \times Q \to Q$, $(g,q) \mapsto \phi(g,q)$. Consider now the cotangent lift of this action, $\tilde{\phi} : G \times T^*Q \to T^*Q$, $(g, p_q) \mapsto \tilde{\phi}(g, p_q) \equiv \phi^*_{g^{-1}} p_q$, where in local coordinates we have

$$\tilde{\phi}(g, p_q) = \left(\phi^i(g^{-1}, q), \frac{\partial \phi^j}{\partial q^i}(g,q) p_j\right).$$

We can define the infinitesimal generators in an analogous manner, by using a curve in G generated by an element $\xi \in \mathfrak{g}$, so that

$$\xi_{T^*Q}(p_q) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\phi}(g(t), p_q)\right|_{t=0}.$$

With this we can define the (Hamiltonian) momentum map $J : T^*Q \to \mathfrak{g}^*$ by

$$\langle J(p_q), \xi\rangle_{\mathfrak{g}} = \langle \theta_Q, \xi_{T^*Q}\rangle = \imath_{\xi_{T^*Q}} \theta_Q$$

where θ_Q is the tautological 1-form. Note that, contrary to the Lagrangian side, this is defined independently of a Hamiltonian. Even better, the cotangent lifted action always satisfies that

$$\tilde{\phi}_g^* \theta_Q = \theta_Q,$$

which means that the momentum map is *always* equivariant, that is

$$J \circ \tilde{\phi}_g = \mathrm{Ad}^*_{g^{-1}} \circ J.$$

Clearly, it also means that

$$\mathcal{L}_{\xi_{T^*Q}} \theta_Q = 0, \tag{3.6}$$

which is its infinitesimal version.

The Hamiltonian version of Noether's theorem states that if H is G-invariant, i.e. $H \circ \tilde{\phi}_g = H$, $\forall g \in G$, then the corresponding momentum map J is conserved, that is, $J \circ F_H^t = J$ for all t. This is easy to see: Let us fix a $\xi \in \mathfrak{g}$,

$$\begin{aligned} X_H(J^\xi) &= \imath_{X_H} \mathrm{d} J^\xi \\ &= \imath_{X_H} \mathrm{d}\left(\imath_{\xi_{T^*Q}} \theta_Q\right) \\ &= \imath_{X_H}\left(\mathcal{L}_{\xi_{T^*Q}} \theta_Q + \imath_{\xi_{T^*Q}} \omega_Q\right) \\ &= -\imath_{\xi_{T^*Q}} \imath_{X_H} \omega_Q \\ &= -\imath_{\xi_{T^*Q}} \mathrm{d} H \end{aligned}$$

where we have made use of Cartan's magic formula and eq.(3.6). Now, one only ought to realize that $\imath_{\xi_{T^*Q}} \mathrm{d}H = \mathcal{L}_{\xi_{T^*Q}} H$ is precisely the infinitesimal version of H being G-invariant and so it must vanish.

Remark. Note that if we also apply Cartan's magic formula to eq.(3.6), we get

$$\imath_{\xi_{T^*Q}} \omega_Q = \mathrm{d}\left(\imath_{\xi_{T^*Q}} \theta_Q\right),$$

which means that ξ_{T^*Q} is always a Hamiltonian vector field ($\tilde{\phi}$ is then said to be a Hamiltonian action), and in particular, in the conditions of Noether's theorem it is *the* Hamiltonian vector field for the corresponding conserved quantity. △

Symplectic reduction

A very interesting and powerful result by Marsden and Weinstein [MW74; AM78] tells us that under certain conditions, if we have a group G acting on a symplectic manifold S, then it may be possible to move to a lower dimensional space formed by the orbits of the group and have that space be a manifold.

Let G act on (S, ω) with a Hamiltonian action, and assume we have an equivariant momentum map $J : S \to \mathfrak{g}^*$. Let $\mu \in \mathfrak{g}^*$ be a regular value of J and denote by G_μ the isotropy group of this value. The theorem states that if G_μ, under the Ad^*-action on $\mathfrak{g}^*$, acts freely and properly on $J^{-1}(\mu)$, then $J^{-1}(\mu)$ is a manifold and there is a unique symplectic form ω_μ, $\pi^*\omega_\mu = i_\mu^* \omega$, with $i_\mu : J^{-1}(\mu) \hookrightarrow S$. That is, $(J^{-1}(\mu)/G_\mu, \omega_\mu)$ is a symplectic manifold [Hos].

In general, if the quotient S/G is a manifold, it may not have the right dimensions to be a symplectic manifold but it will inherit an associated Poisson structure.

If we have a Hamiltonian problem with symmetries in the higher-dimensional manifold, we can then solve it in the quotient and reconstruct the solution in the original space. We will not delve any deeper into the theory, but this is the process which we will apply to many problems in the Lie group setting. There our symplectic manifold will be the cotangent bundle of a group or its tangent bundle equipped with a suitable Poincaré-Cartan symplectic 2-form, and the group will act on itself.

3.1.3 Hamilton-Pontryagin action

In this section we will present the Hamilton-Pontryagin action and its corresponding variational principle. The name was first used in [YM06], but the idea had already been around long before that [see Haa61; Wha90]. At its core, it is a Lagrangian method to

obtain the dynamics of a mechanical system, but it provides an interesting point of view on the relation between the Hamiltonian and the Lagrangian formalism. Moreover, it will play an important role in the construction of numerical methods [e.g., see BM09; KMS10, for some uses].

First, consider the space of curves

$$\begin{aligned} &C^1((q_a, v_a, p_a), (q_b, v_b, p_b), [t_a, t_b]) \\ &= \big\{(q, v, p) : [t_a, t_b] \to \mathbb{T}Q \,|\, q \in C^2([t_a, t_b]), v, p \in C^1([a, b]), \\ &\quad (q, v, p)(t_a) = (q_a, v_a, p_a), (q, v, p)(t_b) = (q_b, v_b, p_b)\big\} \end{aligned}$$

where $\mathbb{T}Q = TQ \oplus T^*Q = \big\{(v_q, \alpha_q), v_q \in T_qQ, \alpha_q \in T_q^*Q, \forall q \in Q\big\}$ denotes the Whitney sum of the tangent and cotangent bundles of Q.

Let us denote by $\pi_\oplus : \mathbb{T}Q \to Q$ the corresponding bundle projection, $\pi_\oplus(v_q, \alpha_q) = q$. Then if $c \in C^1((q_a, v_a, p_a), (q_b, v_b, p_b), [t_a, t_b])$ and $\pi_\oplus c \in C^2(q_a, q_b, [t_a, t_b])$, we say that c is over the curve q.

Let $\mathcal{J}_{\mathcal{HP}} : C^1((q_a, v_a, p_a), (q_b, v_b, p_b), [t_a, t_b]) \to \mathbb{R}$ denote the functional defined by:

$$\mathcal{J}_{\mathcal{HP}}[(q, v, p)] = \int_0^h [L(q(t), v(t)) + \langle p(t), \dot{q}(t) - v(t)\rangle] \,\mathrm{d}t \,. \tag{3.7}$$

This is the so-called **Hamilton-Pontryagin action** functional and it can be interpreted as a constrained functional with p as Lagrange multipliers allowing us to impose the kinematic constraint $\dot{q}(t) = v(t)$. It can be checked that the necessary conditions for the extended curve $c = (q, v, p) \in C^1((q_a, v_a, p_a), (q_b, v_b, p_b), [t_a, t_b])$ to be an admissible critical point of the action, $\mathrm{d}\mathcal{J}_{\mathcal{HP}}[c] = 0$, reduce to the set of equations

$$\begin{aligned} \frac{\mathrm{d}p(t)}{\mathrm{d}t} &= D_1 L(q(t), v(t)), \\ p(t) &= D_2 L(q(t), v(t)), \\ \frac{\mathrm{d}q(t)}{\mathrm{d}t} &= v(t), \quad \forall t \in [0, h]. \end{aligned}$$

These imply that $\pi_\oplus c$ must be a critical point of $\mathcal{J}[q]$, which is not surprising, but they also tell us that the Lagrange multipliers enforcing the constraint are precisely the canonical momenta, hence the notation.

Incidentally, if variations are taken without imposing fixed end-point conditions, we obtain the expected boundary terms

$$\langle p(t), \delta q(t)\rangle|_0^h = \langle p(h), \delta q(h)\rangle - \langle p(0), \delta q(0)\rangle = \theta_L(\delta q)(h) - \theta_L(\delta q)(0).$$

3.1.4 Hamilton-Jacobi theory

The Hamilton-Jacobi equation is a first-order partial differential equation for some function $\bar{S}$ of the general form

$$H\left(t, q^i, \frac{\partial \bar{S}}{\partial q^i}\right) = -\frac{\partial \bar{S}}{\partial t}$$

where $H : \mathbb{R} \times T^*Q \to \mathbb{R}$ is a time-dependent Hamiltonian function. A **complete solution** S is a function dependent on (t, q^i) and $n + 1$ arbitrary constants [see Fer+17;

MMM16, and refs. therein]. As it turns out, it is possible to fix the $n+1$ remaining constants so that they also lie in $\mathbb{R}\times T^*Q$. In this sense, the equation can be rewritten as

$$H\left(t_1, q_1^i, \frac{\partial \bar{S}}{\partial q_1^i}\right) = -\frac{\partial \bar{S}}{\partial t_1}$$

with $\bar{S}(t_0, q_0, t_1, q_1)$, i.e. $\bar{S} : (\mathbb{R}\times T^*Q)\times(\mathbb{R}\times T^*Q)\to\mathbb{R}$.

In the time-independent case the equation simplifies to

$$H\left(q_1^i, \frac{\partial S}{\partial q_1^i}\right) = E,$$

where E is a constant and now $S : T^*Q\times T^*Q\to\mathbb{R}$.

Jacobi found that if H is the Hamiltonian correspondent to a regular Lagrangian L, then the action functional evaluated on solutions of the Euler-Lagrange equations, when interpreted as a function of the boundary values,

$$\mathcal{J}[c] = S(q_0, q_1, T) = \int_0^T L(c(t), \dot{c}(t))\mathrm{d}t, \tag{3.8}$$

with $c\in C^2(q_0, q_1, [0, T])$, is a complete solution of the time-independent Hamilton-Jacobi equation. In fact, this result extends nicely to the time-dependent case, where now

$$\mathcal{J}[c] = \bar{S}(t_0, q_0, t_1, q_1) = \int_{t_0}^{t_1} L(t, c(t), \dot{c}(t))\mathrm{d}t, \tag{3.9}$$

and $c\in C^2(q_0, q_1, [t_0, t_1])$. It is easy to see that this is a solution if we consider the result of eq.(3.1), where we read:

$$\begin{aligned}
\frac{\partial \bar{S}}{\partial q_0}(t_0, q_0, t_1, q_1) &= -\frac{\partial L}{\partial q_0}(t_0, q_0, v_0) = -p_0(t_0, q_0, v_0)\\
\frac{\partial \bar{S}}{\partial t_0}(t_0, q_0, t_1, q_1) &= E_L(t_0, q_0, v_0) = H(t_0, q_0, p_0)\\
\frac{\partial \bar{S}}{\partial q_1}(t_0, q_0, t_1, q_1) &= \frac{\partial L}{\partial q_1}(t_1, q_1, v_1) = p_1(t_1, q_1, v_1)\\
\frac{\partial \bar{S}}{\partial t_1}(t_0, q_0, t_1, q_1) &= -E_L(t_1, q_1, v_1) = -H(t_1, q_1, p_1)
\end{aligned}$$

where $\dot{c}(t_0) = v_0$ and $\dot{c}(t_1) = v_1$.

The geometry behind this is very interesting. The following is taken from [MW01, section 1.4.4] and we will only discuss the time-independent case, although the interpretation is the same in the time-dependent case. Consider $F_H^{\Delta t} : T^*Q\to T^*Q$, the Hamiltonian flow associated with our Hamiltonian H, and consider the graph of this flow, $\mathrm{graph}(F_H^{\Delta t})\subset T^*Q\times T^*Q$, with canonical inclusion $i_{F_H^{\Delta t}} : \mathrm{graph}(F_H^{\Delta t})\to T^*Q\times T^*Q$.

$T^*Q\times T^*Q$ can be equipped with a symplectic structure inherited from T^*Q. If we denote the projections onto the first and second components by $\mathrm{pr}_1, \mathrm{pr}_2 : T^*Q\times T^*Q\to T^*Q$, then we can introduce the 1-form

$$\Theta = \mathrm{pr}_2^*\theta_Q - \mathrm{pr}_1^*\theta_Q,$$

and the symplectic two-form

$$\Omega = -\mathrm{d}\Theta = \mathrm{pr}_2^*\omega_Q - \mathrm{pr}_1^*\omega_Q.$$

Then it is not difficult to show that

$$i^*_{F_H^{\Delta t}}\Omega = \left(F_H^{\Delta t}\right)^* (\mathrm{pr}_2^*\omega_Q - \mathrm{pr}_1^*\omega_Q) = \left(\mathrm{pr}_1|_{\mathrm{graph}(F_H^{\Delta t})}\right)^* \left(\left(F_H^{\Delta t}\right)^*\omega_Q - \omega_Q\right)$$

Note that as $F_H^{\Delta t}$ is symplectic, $\mathrm{graph}(F_H^{\Delta t})$ is a Lagrangian submanifold of $(T^*Q \times T^*Q, \Omega)$ and so $i^*_{F_H^{\Delta t}}\Omega = 0$. This means that $\mathrm{d}\left(i^*_{F_H^{\Delta t}}\Omega\right) = 0$ and by the Poincaré lemma, locally there exists a function $S : \mathrm{graph}(F_H^{\Delta t}) \to \mathbb{R}$ such that $i^*_{F_H^{\Delta t}}\Theta = \mathrm{d}S$.

This result is not only restricted to Hamiltonian flows and can be extended to any symplectic flow. In that context S is said to be a **generating function** of the canonical transformation. Here we have only considered generating functions in $Q \times Q$ but there are other generating functions defined on $T^*Q \times T^*Q$ whose geometric interpretation is more involved.

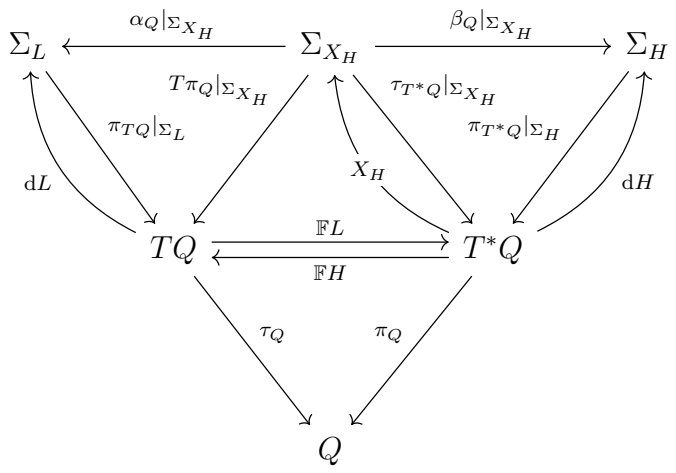
3.1.5 The Tulczyjew's triple in mechanics

In section 2.1.2 we briefly studied the construction by Tulczyjew that relates different double bundles which are at the same time symplectic manifolds [see Tul76a; Tul76b] [see, e.g., GG13; GZ16, for further developments]. This construction provides an intrinsic description of both Lagrangian and Hamiltonian mechanics as Lagrangian submanifolds of these bundles.

Indeed, assume $L : TQ \to \mathbb{R}$ and $H : T^*Q \to \mathbb{R}$ are regular and are related as $H \circ \mathbb{F}L = E_L$. Both functions define sections of their respective double bundles by exterior differentiation, namely $\mathrm{d}L : TQ \to T^*TQ$ and $\mathrm{d}H : T^*Q \to T^*T^*Q$. Let us denote the image of these by $\Sigma_L \subset T^*TQ$ and $\Sigma_H \subset T^*T^*Q$ respectively. The Hamiltonian vector field X_H is also a section $X_H : T^*Q \to TT^*Q$ and we can denote its image by $\Sigma_{X_H} \subset TT^*Q$. Then it can be proved that:

1. Σ_H is a Lagrangian submanifold of (T^*T^*Q, ω_{T^*Q}),
2. Σ_{X_H} is a Lagrangian submanifold of (TT^*Q, ω_α),
3. Σ_L is a Lagrangian submanifold of (T^*TQ, ω_{TQ})
4. $\beta_Q(\Sigma_{X_H}) = \Sigma_H$.
5. $\alpha_Q(\Sigma_{X_H}) = \Sigma_L$.

so we have



3.2 Discrete mechanics and variational integrators

Similar to the continuous case, the discrete Lagrangian description of a mechanical system starts with a choice of the space where the system is going to evolve. Again, this is going to be an n-dimensional configuration manifold Q. The departure from the continuous case comes with the choice of our **state space**, which instead of TQ, will be $Q \times Q$. The interpretation of this is that now each of the copies of Q correspond to different times in the evolution of the system.

The second element necessary to define a discrete Lagrangian system is precisely a **discrete Lagrangian function**. A (time-independent) discrete Lagrangian is a function $L_d : Q \times Q \to \mathbb{R}$, although in order to relate this with the continuous Lagrangian we should probably define it as map $Q \times Q \times \mathbb{R} \to \mathbb{R}$, where the extra argument keeps track of the time scale of the evolution. We will call this the *time-step*, which measures the time elapsed between the first Q component and the second. As we will always work with a fixed time-step, say, $h \in \mathbb{R}$ we will just stick with L_d or use L_d^h if we want to emphasize the step.

A discrete curve on Q can be defined simply as a map $c_d : I_d \subseteq \mathbb{N} \to Q$, although we will prefer to work with time labels $T_d = \{t_i\}_{i=0}^N \in \mathbb{R}$, with $N \in \mathbb{N}$, so that $c_d : T_d \to Q$. A constant step curve is then one where $t_{i+1} - t_i = h, \forall i = 0, ..., N-1$, with time-step h. Consider now the space of discrete curves connecting $q_a, q_b \in Q$.

$$C_d\left(q_a, q_b, T_d\right) = \left\{c_d : T_d \to Q \,|\, c_d(t_a = t_0) = q_a, c_d(t_b = t_N) = q_b\right\}.$$

Its tangent space is then:

$$T_{c_d} C_d\left(q_a, q_b, T_d\right) = \left\{X_d : T_d \to TQ \,|\, \pi_Q X_d = c_d, X_d(t_a = t_0) = X_d(t_b = t_N) = 0\right\}.$$

With this we can define a **discrete action functional**

$$\begin{array}{rccc} \mathcal{J}_d : & C_d\left(q_a, q_b\right) & \longrightarrow & \mathbb{R} \\ & c_d & \longmapsto & \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}), \end{array}$$

as the discrete counterpart of $\mathcal{J}$.

Definition 3.2.1. (Discrete Hamilton's principle). $c_d \in C_d\left(q_a, q_b, T_d\right)$ is a (discrete) physical trajectory of the discrete Lagrangian system defined by a discrete Lagrangian $L_d : Q \times Q \to \mathbb{R}$ if and only if c_d is a critical point of the functional $\mathcal{J}_d$, i.e. $\mathrm{d}\mathcal{J}_d[c_d](X_d) = 0$, for all $X_d \in T_{c_d} C_d(q_a, q_b, T_d)$.

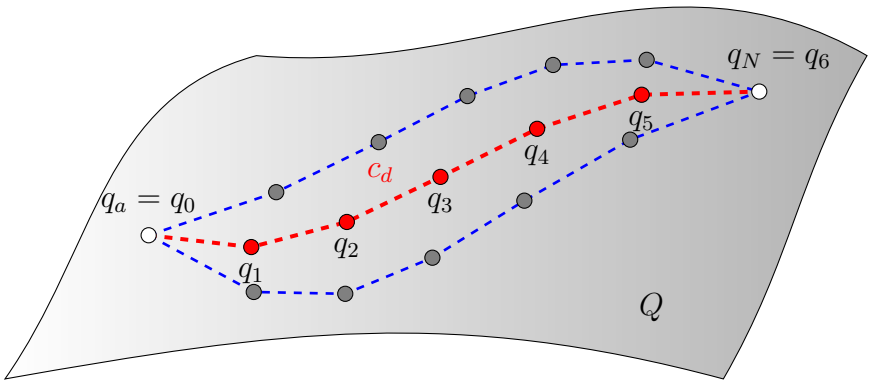
It is easy to show that discrete curves c_d satisfying the discrete Hamilton's principle are the solutions of the following system of implicit difference equations

$$D_2 L_d(q_{i-1}, q_i) + D_1 L_d(q_i, q_{i+1}) = 0, \quad i = 1, ..., N-1; \tag{3.10}$$

These are the *discrete Euler-Lagrange* equations. Each of these equations gives us a map, called a *discrete Lagrangian map*

$$\begin{array}{rccc} F_{L_d} : & Q \times Q & \to & Q \times Q \\ & (q_{i-1}, q_i) & \mapsto & (q_i, q_{i+1}) \end{array}$$

which makes our discrete system evolve, serving as a discrete flow.



Following [MW01], we have that if c_d is a critical point of $\mathcal{J}_d$, then $\mathrm{d}\mathcal{J}_d[c_d] = \Theta^+_{L_d}(q_{N-1}, q_N) - \Theta^-_{L_d}(q_0, q_1) = \left[\left(F^{N-1}_{L_d}\right)^* \Theta^+_{L_d} - \Theta^-_{L_d}\right](q_0, q_1)$, where

$$\begin{aligned} \Theta^-_{L_d}(q_0, q_1) &= -D_1 L_d(q_0, q_1)\mathrm{d}q_0 \\ \Theta^+_{L_d}(q_0, q_1) &= D_2 L_d(q_0, q_1)\mathrm{d}q_1 \end{aligned}$$

are called the discrete Poincaré-Cartan 1-forms. As in the continuous case we can define discrete Poincaré-Cartan 2-forms as $\Omega^\pm_{L_d} = -\mathrm{d}\Theta^\pm_{L_d}$, and as it turns out they coincide, that is

$$\Omega^+_{L_d} = \Omega^-_{L_d} = \Omega_{L_d} = \frac{\partial^2 L_d}{\partial q_0^j \partial q_1^i}\mathrm{d}q_1^i \wedge \mathrm{d}q_0^j.$$

From $\mathrm{d}^2\mathcal{J}_d(c_d) = 0$ we get that

$$\left(F^{N-1}_{L_d}\right)^* \Omega_{L_d} = \Omega_{L_d},$$

which is true for any number of steps. This means that the discrete Lagrangian flow preserves this form.

3.2.1 Discrete fibre derivative

Consider the maps $\mathbb{F}^\pm L_d : Q \times Q \to T^*Q$ defined by

$$\begin{aligned} \mathbb{F}^- L_d(q_0, q_1) &= (q_0, p_0 = -D_1 L_d(q_0, q_1)), \\ \mathbb{F}^+ L_d(q_0, q_1) &= (q_1, p_1 = D_2 L_d(q_0, q_1)). \end{aligned}$$

These are called **discrete fibre derivatives** (or *discrete Legendre transforms*). As in the continuous case we say that the discrete Lagrangian is regular if both discrete fibre derivatives are local diffeomorphisms, which is equivalent to the regularity of the Hessian matrix whose coefficients are

$$(g_{L_d})_{ij} = \frac{\partial^2 L_d}{\partial q_0^i \partial q_1^j}. \tag{3.11}$$

This is equivalent to the non-degeneracy of the discrete Poincaré-Cartan 2-form, Ω_{L_d}, ensuring it is a symplectic form. We will commonly assume that our discrete Lagrangian is regular.

Note that with these discrete fibre derivatives, eqs.(3.10) can be reinterpreted as a **matching condition** for the momenta

$$\begin{gathered}\mathbb{F}^+L_d(q_{k-1},q_k)=\mathbb{F}^-L_d(q_k,q_{k+1})\\ \Updownarrow\\ D_2L_d(q_{k-1},q_k)=p_k^{\rightarrow\bullet}=p_k^{\bullet\leftarrow}=-D_1L_d(q_k,q_{k+1})\end{gathered}$$

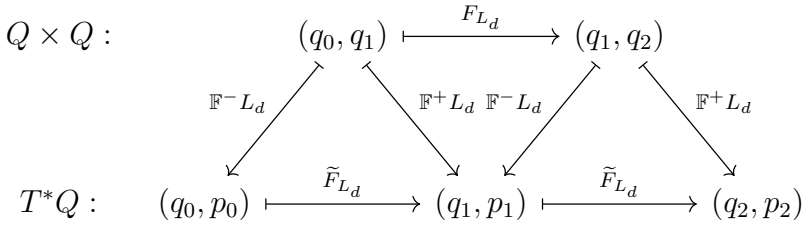
with $k=1,...,N-1$. This can be alternatively written as

$$\mathbb{F}^+L_d=\mathbb{F}^-L_d\circ F_{L_d}.$$

If the Lagrangian is regular, then by the inverse function theorem there exists a unique local function $q_{k+1}(q_{k-1},q_k)$ satisfying the discrete Euler-Lagrange equations. Furthermore, in this case we get that

$$\left(\mathbb{F}^+L_d\right)^*\omega_Q=\left(F_{L_d}\right)^*\left(\mathbb{F}^-L_d\right)^*\omega_Q=\Omega_{L_d}.$$

We can define a flow $\widetilde{F}_{L_d}:T^*Q\to T^*Q$ such that the following diagram commutes,



This map receives the name of *discrete Hamiltonian map* and is also discretely symplectic, that is

$$\widetilde{F}_{L_d}^*\omega_Q=\omega_Q.$$

3.2.2 Discrete Noether's theorem

Let G be a Lie group with Lie algebra $\mathfrak{g}$ and let it act on Q with the action $\phi:G\times Q\to Q$, $(g,q)\mapsto\phi(g,q)$. Consider the diagonal action, $\phi^\times:G\times Q\to Q$, $(g,q_0,q_1)\mapsto\phi^\times(g,q_0,q_1)\equiv(\phi(g,q_0),\phi(g,q_1))$.

If ξ_Q is the infinitesimal generator as defined in section 3.1.1, then we say that $\xi_{Q\times Q}:Q\times Q\to T(Q\times Q)$ is the **discrete infinitesimal generator** of the diagonal action $\phi^\times_{g(t)}$ defined by

$$\xi_{Q\times Q}(q_0,q_1)=(\xi_Q(q_0),\xi_Q(q_1))$$

Theorem 3.2.1 (**Discrete Noether's theorem**). *[MW01, theorem 1.3.2] Let (Q,L_d) define a discrete Lagrangian mechanical system and assume that L_d is invariant under the diagonal action $\phi^\times$ for a curve $g(\epsilon)$ generated by $\xi\in\mathfrak{g}$, that is,*

$$L_d\circ\phi^\times_{g(\epsilon)}=L_d,\quad\forall\epsilon\,.$$

Then

$$\left\langle\Theta^+_{L_d},\xi_{Q\times Q}\right\rangle\circ F^k_{L_d}=\left\langle\Theta^-_{L_d},\xi_{Q\times Q}\right\rangle\,.$$

for all $k=1,...,N-1$.

Proof. Assume c_d is a discrete physical trajectory, i.e.

$$\mathrm{d}\mathcal{J}_d[c_d](X_d) = 0,$$

for all $X_d \in T_{c_d}C_d(q_a, q_b, T_d)$. Choose X_d such that $X_d(t_k) = \xi_Q(c_d(t_k))$, for all $k = 0, ..., N$, so the varied paths can be interpreted as generated by $c_{d,\epsilon}(t_k) = \phi\left(\exp(\epsilon\xi), c_d(t_k)\right)$, where $\exp(\epsilon\xi) = g(\epsilon)$. Note that such a choice of X_d induces a discrete infinitesimal generator under the identification

$$\xi_{Q\times Q}(q_k, q_{k+1}) = (X_d(t_k), X_d(t_{k+1})) = (\xi_Q(q_k), \xi_Q(q_{k+1})), \quad \forall k = 0, ..., N-1$$

This choice means that

$$\mathrm{d}\mathcal{J}_d[c_d](X_d) = \sum_{k=0}^{N-1} \mathrm{d}L_d(q_k, q_{k+1})(\xi_{Q\times Q}) = 0,$$

and as c_d is a discrete physical trajectory, then this is true for each interval, which implies that

$$\left\langle \Theta^+_{L_d}, \xi_{Q\times Q} \right\rangle \circ F_{L_d} = \left\langle \Theta^-_{L_d}, \xi_{Q\times Q} \right\rangle .$$

for every pair (q_k, q_{k+1}) for $k = 0, ..., N-1$, which implies the result of the theorem. □

If we define the **discrete Lagrangian momentum maps**, $J^{\pm}_{L_d} : Q \times Q \to \mathfrak{g}^*$ by the relation

$$\left\langle J^+_{L_d}(q_0, q_1), \xi \right\rangle_{\mathfrak{g}} = \left\langle \Theta^+_{L_d}, \xi_{Q\times Q} \right\rangle,$$
$$\left\langle J^-_{L_d}(q_0, q_1), \xi \right\rangle_{\mathfrak{g}} = \left\langle \Theta^-_{L_d}, \xi_{Q\times Q} \right\rangle,$$

then if L_d is invariant under the diagonal action $\phi^{\times}_g$, we say that under the conditions of the discrete Noether's theorem the discrete momentum map is conserved along the flow.

3.2.3 Correspondence with continuous mechanics and variational integrators

The question now is, given a regular (time-independent) Lagrangian mechanical system (Q, L), can we find a discrete $L_d : Q \times Q \to \mathbb{R}$ whose discrete dynamics correspond to that of the continuous system?

The answer lies in Jacobi's solution to the Hamilton-Jacobi equation, eq.3.8. Let $c \in C^k(q_a, q_b, [t_a, t_b])$, with $k \geq 2$, be a critical point of the functional $\mathcal{J}$. Then $S(q_a, q_b, t_b - t_a) = \mathcal{J}[c]$ is a complete solution of the Hamilton-Jacobi equation.

Let us take the interval $I = [t_a, t_b]$ and divide it into N equal length subintervals $\{I_{k,k+1} = [t_k, t_{k+1}]\}_{k=0}^{N-1}$, with $t_a = t_0$ and $t_b = t_N$ and $h = t_{k+1} - t_k$. This splits the curve c into the curves $\{c_{k,k+1} = c(I_{k,k+1})\}_{i=0}^{N-1}$ with $c_{k,k+1} \in C^k(q_k, q_{k+1}, I_{k,k+1})$ and $q_0 = q_a, q_N = q_b$. It is not difficult to see that $S(q_k, q_{k+1}) \equiv S(q_k, q_{k+1}, h) = \mathcal{J}[c_{k,k+1}]$, with $c_{k,k+1}$ a critical point.

Now, clearly, $c_d = c(T_d)$, with $T_d = \{t_k\}_{k=0}^N$ must be a discrete curve belonging to $C_d(q_a, q_b, T_d)$. Furthermore, it can immediately be seen that c_d is a critical point of the discrete action $\mathcal{J}_d$ defined by the discrete Lagrangian

$$L^e_d(q_k, q_{k+1}) = \int_{t_k}^{t_{k+1}} L(\hat{c}_{k,k+1}(t))\mathrm{d}t = S(q_k, q_{k+1}), \quad \forall k = 1, ..., N-1\,,$$

where $\hat{c}_{k,k+1}$ is the tangent lift of the curve $c_{k,k+1}$.

As we are working in the time-independent case, it is possible to reparametrize the curves so that we can write

$$L_d^e(q_k, q_{k+1}) = \int_0^h L(\hat{c}_{k,k+1}(t(\tau)))\mathrm{d}\tau, \quad \forall k = 1, ..., N-1.$$

We say that this discrete Lagrangian is **exact** in the sense that it reproduces the dynamics of L in a discrete sense exactly. Results from the theory of calculus of variations [see Ber12] and from the theory of ODEs [see Har02, chapter 4.4] guarantee that if the step h is small enough and L regular, then L_d^e *exists and is unique* [see MMM16].

Proposition 3.2.1. *Let $L : TQ \to \mathbb{R}$ be a regular Lagrangian. Then there exists a deleted neighborhood of 0, $U_0^* = U_0 \setminus \{0\}$, with $U_0 \subseteq \mathbb{R}$, for which the exact discrete Lagrangian, $L_d^{h,e} \equiv L_d^e$, with $h \in U_0^*$, is regular.*

Proof. If L_d^e is regular, then the Hessian matrix $g_{L_d^e}$ defined in eq.(3.11) must be regular. We know that

$$\frac{\partial L_d^e}{\partial q_0^i} = \sum_{j=1}^n \frac{\partial L}{\partial \dot{q}^j}(q(t), \dot{q}(t))\frac{\partial q^j}{\partial q_0^i}(t)\bigg|_0^h = -\frac{\partial L}{\partial q^i}(q(0), \dot{q}(0))$$

where we have used that $q^i(0) = q_0^i$.

$$\begin{aligned}
\frac{\partial^2 L_d^e}{\partial q_0^i \partial q_1^j} &= \frac{\partial}{\partial q_1^j}\left(\sum_{k=1}^n \frac{\partial L}{\partial \dot{q}^k}(q(t), \dot{q}(t))\frac{\partial q^k}{\partial q_0^i}(t)\right)\bigg|_0^h \\
&= \left(\sum_{k,l=1}^n \frac{\partial^2 L}{\partial \dot{q}^k \partial q^l}(q(t), \dot{q}(t))\frac{\partial q^k}{\partial q_0^i}(t)\frac{\partial q^l}{\partial q_1^j}(t)\right)\bigg|_0^h \\
&+ \left(\sum_{k,l=1}^n \frac{\partial^2 L}{\partial \dot{q}^k \partial \dot{q}^l}(q(t), \dot{q}(t))\frac{\partial q^k}{\partial q_0^i}(t)\frac{\partial \dot{q}^l}{\partial q_1^j}(t)\right)\bigg|_0^h \\
&+ \left(\sum_{k=1}^n \frac{\partial L}{\partial \dot{q}^k}(q(t), \dot{q}(t))\frac{\partial^2 q^k}{\partial q_0^i \partial q_1^j}(t)\right)\bigg|_0^h \\
&= -\sum_{l=1}^n \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^l}(q(0), \dot{q}(0))\frac{\partial \dot{q}^l}{\partial q_1^j}(0)
\end{aligned}$$

where the first and the third term vanish because

$$\begin{aligned}
\frac{\partial q}{\partial q_0}(0) = I_n, \quad \frac{\partial q}{\partial q_1}(0) = 0, \\
\frac{\partial q}{\partial q_0}(h) = 0, \quad \frac{\partial q}{\partial q_1}(h) = I_n.
\end{aligned}$$

What remains is to analyze $\frac{\partial \dot{q}}{\partial q_1}(0)$, but a simple estimate $q_1^i = q_0^i + h\dot{q}^i + \mathcal{O}(h^2)$ tells us that the lowest order term must be $\frac{1}{h}I_n$, so

$$\frac{\partial^2 L_d^e}{\partial q_0^i \partial q_1^j} = -\frac{1}{h}\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}(q(0), \dot{q}(0)) + \mathcal{O}(1),$$

which in turn implies the result of the proposition. □

Although warranted to exist, it is generally not possible to obtain an analytic closed-form expression for the exact discrete Lagrangian. Instead, what we can do is try to approximate the action integral by some *quadrature rule* in hopes that the extremum of this approximation converges to the extremum of the continuous problem as the quality of our quadrature augments and as the length of our intervals, h, diminishes. This leads to the following definition:

Definition 3.2.2. Let $L_d : Q \times Q \to \mathbb{R}$ be a discrete Lagrangian. We say that L_d is a **discretization of order** r if there exist an open subset $U_1 \subset TQ$ with compact closure and constants $C_1 > 0$, $h_1 > 0$ so that:

$$\|L_d(q(0), q(h)) - L_d^e(q(0), q(h))\| \leq C_1 h^{r+1}$$

for all solutions $q(t)$ of the second-order Euler-Lagrange equations with initial conditions $(q_0, \dot{q}_0) \in U_1$ and for all $h \leq h_1$.

This means that, given a discrete Lagrangian L_d, its order can be calculated by expanding the expressions for $L_d(q(0), q(h))$ in a Taylor series in h and comparing this to the same expansions for the exact Lagrangian. If the series agree up to r terms, then the discrete Lagrangian is of order r.

Using our approximations $L_d \approx L_d^e$ we can apply the discrete Hamilton's principle, which leads us again to eq.(3.10). The resulting discrete flows, be it the discrete Lagrangian map F_{L_d} or the discrete Hamiltonian map $\widetilde{F}_{L_d}$, become our **variational integrator**. By construction, variational integrators automatically preserve symplecticity, as we have seen, and thus they are *symplectic integrators*. They also preserve momentum and exhibit quasi-energy conservation for exponentially long times [cf. MW01; HLW10, and refs. therein].

Following [MW01; PC09], we have the next result about the order of a variational integrator, which confirms our crude supposition about convergence.

Theorem 3.2.2 (**Variational error**). *Let $\widetilde{F}_{L_d} : T^*Q \to T^*Q$ be the Hamiltonian map of the regular discrete Lagrangian $L_d : Q \times Q \to \mathbb{R}$. Then, if L_d is of order r, this implies that*

$$\widetilde{F}_{L_d} = \widetilde{F}_{L_d^e} + \mathcal{O}(h^{r+1}).$$

This result is key as it essentially tells us that the order of the quadrature rule we use to approximate our discrete Lagrangian will be the order of the resulting variational integrator.

Remark (1). The original result by J. Marsden and M. West in [MW01] stated a triple equivalence between the order of L_d and the order of the flow, $\widetilde{F}_{L_d}$, together with the order of the fibre derivative, $\mathbb{F}^{\pm}L_d$. Later G. Patrick and C. Cuell in [PC09] showed that this triple equivalence was not true, the culprit being in part the singularity of the discrete Lagrangian at $h = 0$. They found that the order of the discrete fibre derivative could indeed be lower than r, yet it could lead to flows of order r. Interestingly this result does not invalidate the result that

$$\mathbb{F}^+L_d = \mathbb{F}^-L_d \circ F_{L_d}\,,$$

so the discrete Euler-Lagrange equations are still a matching of momenta, but both may contain symmetric spurious terms that do not affect the end result. △

Remark (2). An important point to make here is that we are considering the *Hamiltonian flow*. If we want to use a variational integrator to obtain an approximate solution to an IVP for some Lagrangian L with initial value $(q_0, v_0) \in TQ$, we need to choose appropriate initial conditions for our method.

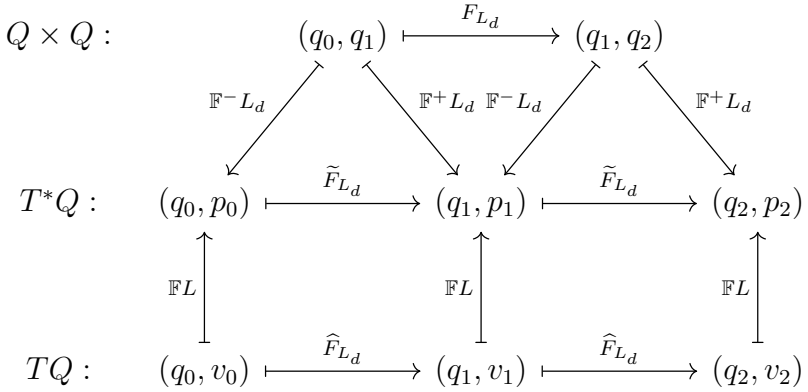
Note that F_{L_d} needs initial values $(q_0, q_1) \in Q \times Q$ and $\widetilde{F}_{L_d}$ needs initial values $(q_0, p_0) \in T^*Q$. Starting directly with values in $Q \times Q$ by providing an external estimate of q_1 is never a good idea, but it is unfortunately a prevalent one. Even worse, the same mistake can and is repeated when retrieving the numerical solution given by the variational integrator, leading to even more problems that hurt the convergence.

The canonical way to deal with this problem is to use the continuous fibre derivative to sidestep the issue. In fact, if we denote as $\widehat{F}_{L_d} : TQ \to TQ$ the map defined by $\widehat{F}_{L_d} = (\mathbb{F}L)^{-1} \circ \widetilde{F}_{L_d} \circ \mathbb{F}L$, we see that the result of the theorem must be true for it too, that is

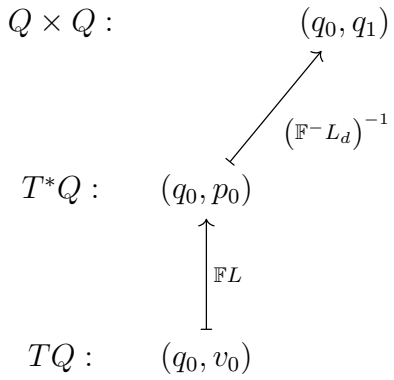
$$\widehat{F}_{L_d} = F_L^h + \mathcal{O}(h^{r+1}),$$

where we note that

$$\widehat{F}_{L_d^e} = F_L^h,$$



This way, in order to start our variational integrators on $Q \times Q$ we should always transform the initial conditions as $\left[(\mathbb{F}^- L_d)^{-1} \circ \mathbb{F}L\right](q_0, v_0) \in Q \times Q$:



△

3.2.4 Symplectic integrators and energy

As we have seen, variational integrators are automatically symplectic. However, an important result from Ge and Marsden [Ge91; ZM88] shows that a fixed-step symplectic integrator cannot preserve energy unless it is exact (up to a reparametrization of time).

So why care about symplecticity instead of energy conservation when the latter is such a big part of mechanics? The answer lies in the following result proposed by A. Murua in his thesis [Mur95] and in [BG94]. The version here is a slightly modified version of the one in [HLW10, theorem IX.3.2, p.345].

Theorem 3.2.3. *Assume that the symplectic method with discrete flow $\tilde{\Phi}_h : T^*Q \to T^*Q$ has a generating function*

$$S(p_1, q_0, h) = S_0(p_1, q_0) + hS_1(p_1, q_0) + h^2 S_2(p_1, q_0) + h^3 S_3(p_1, q_0) + ...$$

where (q_0, p_0, q_1, p_1) are local coordinates in $T^*Q \times T^*Q$, with smooth $S_j(p_1, q_0)$ defined on an open set $\bar{U} \subseteq T^*Q \times T^*Q$ such that $\mathrm{pr}_i(\bar{U}) = U$, $i = 1, 2$, and where

$$p_1 = D_1 S_0(p_1, q_0), \quad q_0 = D_2 S_0(p_1, q_0).$$

Then, the modified differential equation whose flow coincides with $\tilde{\Phi}_h$, is a Hamiltonian system with

$$\tilde{H} = H + hH_2 + h^3 H_3 + ...$$

where the functions $H_j = H_j(q, p)$ are defined and smooth on the whole U.

Remark. Here the function S is a generating function of the more general form that was commented in the last part of section 3.1.4. As a generating function it must then satisfy

$$p_0 = D_1 S(p_1, q_0), \quad q_1 = D_2 S(p_1, q_0). \qquad \triangle$$

In short, this result proves through backward error analysis that the discrete flow of a symplectic integrator, $\tilde{\Phi}_h$ (which in the case of our variational integrators we denoted as $\widetilde{F}^h_{L_d}$), is globally Hamiltonian. This in turn means that it is the exact flow of a certain modified Hamiltonian, $\tilde{H}$, that is close to the original Hamiltonian H [SC94].

In Lagrangian terms this implies that even if we are not exactly preserving the energy of our system, we are indeed preserving a *modified energy* exactly, and this modified energy will be as close to the exact energy as the discrete flow is close to the exact flow. This result explains one of the main qualitative features of symplectic integrators: good *long-term energy behavior*. Whereas general purpose non-symplectic integrators tend to display some form of energy drift, be it decay (energy dissipation) or growth (energy gain), symplectic integrators display quasi-conservation, that is, the energy remains bounded and close to the exact energy.

The bottom line is that when using a symplectic integrator we can have geometric correctness in the form of symplecticity (which itself leads to good statistical properties), momentum conservation and quasi-energy conservation.

3.2.5 Generation of high-order variational integrators

In previous sections we have seen that we can construct variational integrators by generating a discrete Lagrangian that approximates the discrete critical action, that is, the exact discrete Lagrangian. Assuming Q is a vector space, one of the first methods one can think of is to use a simple numerical integration rule such as the midpoint rule (1-stage Gauss) or the trapezoidal rule (2-stage Lobatto). These result in

$$L_d(q_0, q_1) = hL\left(\frac{q_1 + q_0}{2}, \frac{q_1 - q_0}{h}\right),$$
$$L_d(q_0, q_1) = \frac{h}{2}L\left(q_0, \frac{q_1 - q_0}{h}\right) + \frac{h}{2}L\left(q_1, \frac{q_1 - q_0}{h}\right),$$

respectively, which are both order 2 methods.

Now, to generate high-order methods, that is, methods of order $p > 2$, there are a number of options. One of them is the use of composition [see HLW10; MW01, for additional information], which allows us to increase the order by mixing different size steps of a lower order method to create a higher order step.

Another option is to find an approximation to the solution curve in a space of polynomials of degree r [MW01; Leo04; Obe17]. For each step k we have an approximation curve $q_d(d_i, q_k^i) : [0, h] \to Q$ parametrized by $r + 1$ control points. These control points are defined by their respective temporal and spatial position specified by a set of fixed values $0 = d_0 < d_1 < ... < d_r = 1$ and free $\{q_k^i \in Q\}_{i=0}^r$ respectively, so that we can write

$$q_d(d_i, q_k^i, h\tau) = \sum_{j=0}^{r} q_k^j \ell_j(\tau)$$

where $l_j(\tau)$ is the i-th element of the Lagrange basis of dimension $r + 1$ (polynomials of order r) associated with the d_i coefficients. Thus, the approximation satisfies

$$q_d(d_i, q_k^i, d_j h) = q_k^j \,.$$

One then chooses a suitable quadrature rule (b_i, c_i) of order s to approximate the exact discrete Lagrangian as

$$L_d(q_k^i) = h \sum_{i=1}^{s} b_i L(q_d(d_i, q_k^i, c_i h), \dot{q}_d(d_i, q_k^i, c_i h))$$

where, in order to approximate the velocities, we differentiate q_d with respect to time. The action for the entire interval is then

$$\mathcal{J}_d[c_d] = \sum_{k=0}^{N-1} L_d(q_k^i)$$

together with constraints to enforce that $q_k^r = q_{k+1}^0$. Applying the discrete Hamilton's principle we get the equations

$$\begin{aligned} D_{r+1} L_d(q_{k-1}^i) + D_1 L_d(q_k^i) &= 0, \\ D_j L_d(q_k^i) &= 0, \quad \forall j = 2, ..., r \,. \end{aligned}$$

Methods of this form are called Galerkin methods. The two order 2 methods in the form stated above fall precisely in this category with linear polynomials and $d_0 = 0$, $d_1 = 1$ and their respective quadratures. This approach is certainly easy to implement and tends to give accurate results.

The last option we will discuss will be of central importance in a good part of this work (chapter 5). The idea is to use general Runge-Kutta (RK) methods in the generation of our discrete Lagrangian, but initially it might not be clear how to do so. The key is to start not from the standard action but from the Hamilton-Pontryagin action. This will lead us to variationally partitioned RK methods.

The first thing to do is to discretize the constraint $\dot{q} = v$. Assuming we are working on a vector space Q (later we will explore the case of a Lie group), we can do so by using an s-stage RK scheme for the integration of such an ODE:

$$Q_0^i = q_0 + h\sum_{j=1}^{s} a_{ij} V_0^i\,, \qquad q_1 = q_0 + h\sum_{j=1}^{s} b_j V_0^i\,.$$

It will be assumed that the method is of order $p > 1$, and thus it satisfies the order 1 condition

$$\sum_{j=1}^{s} b_j = 1. \tag{order 1}$$

Following [BM09], given the chosen s-stage RK scheme with $T_d = \{t_k\}_{k=0}^N$ such that $t_{k+1} - t_k = h$, let us consider the space of *s-stage variationally partitioned RK (s-stage VPRK) sequences*:

$$\begin{aligned} &C_d^s(q_a, q_b) \\ &= \left\{ \left(q, \tilde{p}, \left\{ Q^i, V^i, \tilde{P}^i \right\}_{i=1}^{s} \right) : T_d \to T^*Q \times (\mathbb{T}Q)^s \mid q(a) = q_a, q(b) = q_b \right\}. \end{aligned}$$

Then we can define the following discrete Hamilton-Pontryagin functional / extended cost functional $(\mathcal{J}_{\mathcal{HP}})_d : C_d^s(q_a, q_b) \to \mathbb{R}$, by:

$$\begin{aligned} (\mathcal{J}_{\mathcal{HP}})_d [c_d] = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h b_i \Bigg[& L\left(Q_k^i, V_k^i\right) + \left\langle \tilde{P}_k^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle \\ & + \left\langle \tilde{p}_{k+1}, \frac{q_{k+1} - q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle \Bigg] \end{aligned} \tag{3.12}$$

Theorem 3.2.4. *Let $L : TQ \to \mathbb{R}$ be a C^ℓ function with $\ell \geq 2$ and an s-stage VPRK sequence $c_d \in C_d^s(q_0, q_N)$. Then c_d is a critical point of the discrete Hamilton-Pontryagin functional, $(\mathcal{J}_{\mathcal{HP}})_d$, if and only if for all $k = 0, ..., N-1$ and $i = 1, ..., s$ it satisfies*

$$\begin{array}{ll} q_{k+1} = q_k + h\sum_{j=1}^{s} b_j V_k^j, & p_{k+1} = p_k + h\sum_{i=1}^{s} \hat{b}_j W_k^j, \\ Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, & P_k^i = p_k + h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \\ W_k^i = D_1 L(Q_k^i, V_k^i), & P_k^i = D_2 L(Q_k^i, V_k^i), \end{array} \tag{3.13}$$

where the RK coefficients satisfy $b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j$ and $\hat{b}_i = b_i$.

The condition on the RK coefficients is called the *symplecticity condition* of the partitioned method (see section 2.3.1).

Proof. Computing the variations of this action we get:

$$\begin{aligned} &\left\langle \mathrm{d}\left(\mathcal{J}_{\mathcal{HP}}\right)_d, \delta c_d \right\rangle \\ &\quad = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h b_i \Bigg[\left\langle D_1 L\left(Q_k^i, V_k^i\right), \delta Q_k^i \right\rangle + \left\langle D_2 L\left(Q_k^i, V_k^i\right), \delta V_k^i \right\rangle \\ &\quad + \left\langle \delta \tilde{P}_k^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle + \left\langle \tilde{P}_k^i, \frac{\delta Q_k^i - \delta q_k}{h} - \sum_{j=1}^{s} a_{ij} \delta V_k^j \right\rangle \\ &\quad + \left\langle \delta \tilde{p}_{k+1}, \frac{q_{k+1} - q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle + \left\langle \tilde{p}_{k+1}, \frac{\delta q_{k+1} - \delta q_k}{h} - \sum_{j=1}^{s} b_j \delta V_k^j \right\rangle \Bigg] \end{aligned}$$

Let us collect all the different terms separately:

$$\begin{aligned}
\delta q : \sum_{k=0}^{N-1}\sum_{i=1}^{s} b_i \left[-\left\langle \tilde{P}_k^i, \delta q_k \right\rangle + \langle \tilde{p}_{k+1}, \delta q_{k+1} - \delta q_k \rangle \right] \\
= \sum_{k=0}^{N-1}\sum_{i=1}^{s} b_i \left[-\left\langle \tilde{P}_k^i + \tilde{p}_{k+1}, \delta q_k \right\rangle + \langle \tilde{p}_{k+1}, \delta q_{k+1} \rangle \right] \\
= \sum_{k=1}^{N-1}\sum_{i=1}^{s} b_i \left[\left\langle -\tilde{P}_k^i + \tilde{p}_k - \tilde{p}_{k+1}, \delta q_k \right\rangle \right] \\
+ \sum_{i=1}^{s} b_i \langle \tilde{p}_N, \delta q_N \rangle - \sum_{i=1}^{s} b_i \left\langle \tilde{P}_0^i + \tilde{p}_1, \delta q_0 \right\rangle \\
= \sum_{k=1}^{N-1} \left\langle \tilde{p}_k - \tilde{p}_{k+1} - \sum_{i=1}^{s} b_i \tilde{P}_k^i, \delta q_k \right\rangle \\
+ \langle \tilde{p}_N, \delta q_N \rangle - \left\langle \sum_{i=1}^{s} b_i \tilde{P}_0^i + \tilde{p}_1, \delta q_0 \right\rangle
\end{aligned}$$

where we have used the order 1 condition.

$$\begin{aligned}
\delta Q : \sum_{k=0}^{N-1}\sum_{i=1}^{s} b_i \left[\left\langle hD_1 L\left(Q_k^i, V_k^i\right), \delta Q_k^i \right\rangle + \left\langle \tilde{P}_k^i, \delta Q_k^i \right\rangle \right] \\
= \sum_{k=0}^{N-1}\sum_{i=1}^{s} b_i \left\langle hD_1 L\left(Q_k^i, V_k^i\right) + \tilde{P}_k^i, \delta Q_k^i \right\rangle
\end{aligned}$$

$$\begin{aligned}
\delta V : \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left[\left\langle D_2 L\left(Q_k^i, V_k^i\right), \delta V_k^i \right\rangle - \left\langle \tilde{P}_k^i, \sum_{j=1}^{s} a_{ij} \delta V_k^j \right\rangle - \left\langle \tilde{p}_{k+1}, \sum_{j=1}^{s} b_j \delta V_k^j \right\rangle \right. \\
\left. - \left\langle \sum_{i=1}^{s} b_i \tilde{p}_{k+1}, \sum_{j=1}^{s} b_j \delta V_k^j \right\rangle \right] \\
= \sum_{k=0}^{N-1} h \left[\left\langle \sum_{i=1}^{s} b_i D_2 L\left(Q_k^i, V_k^i\right), \delta V_k^i \right\rangle - \sum_{i=1}^{s}\sum_{j=1}^{s} \left\langle b_j \tilde{P}_k^j, a_{ji} \delta V_k^i \right\rangle \right. \\
\left. - \left\langle \tilde{p}_{k+1}, \sum_{i=1}^{s} b_i \delta V_k^i \right\rangle \right] \\
= \sum_{k=0}^{N-1}\sum_{i=1}^{s} h \left\langle b_i D_2 L\left(Q_k^i, V_k^i\right) - \sum_{j=1}^{s} b_j a_{ji} \tilde{P}_k^j - b_i \tilde{p}_{k+1}, \delta V_k^i \right\rangle
\end{aligned}$$

$$\delta \tilde{p} : \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \delta \tilde{p}_{k+1}, \frac{q_{k+1} - q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle$$

$$\delta\tilde{P} : \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \delta\tilde{P}_k^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij}V_k^j \right\rangle$$

From these last two variations we recuperate the original discrete kinematic constraints, as expected.

From δQ we get that

$$\tilde{P}_k^i = -hD_1L\left(Q_k^i, V_k^i\right) .$$

Inserting this in δq we obtain:

$$\tilde{p}_{k+1} = \tilde{p}_k + h\sum_{i=1}^{s} b_i D_1L\left(Q_k^i, V_k^i\right) .$$

Comparing the boundary terms from the continuous and discrete cases we see that these $\tilde{p}_k$ variables are approximations to the continuous $p(t_k)$. Thus, we will drop the tildes, making this identification explicit.

From δV we find that:

$$D_2L\left(Q_k^i, V_k^i\right) = p_{k+1} - h\sum_{j=1}^{s} \frac{b_j a_{ji}}{b_i} D_1L\left(Q_k^j, V_k^j\right)$$

Inserting what we found from δq here, we get:

$$D_2L\left(Q_k^i, V_k^i\right) = p_k + h\sum_{j=1}^{s} b_j \left(1 - \frac{a_{ji}}{b_i}\right) D_1L\left(Q_k^j, V_k^j\right)$$

Rewriting the equations using $\hat{b}_i$, $\hat{a}_{ij}$, P_k^i and W_k^i we get the result we were after. □

The resulting system of equations from theorem 3.2.4 defines a discrete Hamiltonian map, i.e. a mapping $(q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$ and in order to determine these we will also need to determine the set $\{Q_k^i, V_k^i\}_{i=1}^s$. By theorem 3.2.2, the order of the discrete Hamiltonian map will coincide with the order of the RK method applied [HLW10; MW01; PC09].

The first order 2 method shown above can also be thought of as the corresponding VPRK for the 1-stage Gauss, and if the Lagrangian is such that g_L is constant, then the second can also be interpreted as the corresponding VPRK method for the 2-stage Lobatto IIA. This should not be surprising, as both are continuous collocation methods and the idea behind this type of RK methods and that of Galerkin methods is certainly very similar (though the order of the polynomials differs).

It should be noted that defining the set $\{v_k\}_{k=0}^N$ by the relation $p_k = D_2L(q_k, v_k)$, we can rewrite the integrator to obtain a discrete Lagrangian flow $\widehat{F}_{L_d} : TQ \to TQ$, $(q_k, v_k) \mapsto (q_{k+1}, v_{k+1})$

$$\begin{aligned} q_{k+1} &= q_k + h\textstyle\sum_{j=1}^{s} b_j V_k^j, & D_2L(q_{k+1}, v_{k+1}) &= D_2L(q_k, v_k) + h\textstyle\sum_{i=1}^{s} \hat{b}_j D_1L(Q_k^j, V_k^j), \\ Q_k^i &= q_k + h\textstyle\sum_{j=1}^{s} a_{ij} V_k^j, & D_2L(Q_k^i, V_k^i) &= D_2L(q_k, v_k) + h\textstyle\sum_{j=1}^{s} \hat{a}_{ij} D_1L(Q_k^j, V_k^j), \end{aligned} \tag{3.14}$$

3.3 Mechanics on Lie groups

When our configuration manifold is a Lie group G, we have the natural action of the group acting on itself [AM78; MR99; Hol11a; Hol11b]. This allows us to trivialize using the left (or right, alternatively) translation and even apply reduction theory to simplify the problems. Here what is meant by **trivialization** is the use of the mappings

$$\begin{aligned} TG \to G \times \mathfrak{g} \ , \qquad & (g, \dot{g}) \mapsto (g, (T_g L_{g^{-1}})\dot{g}) = (g, \eta) \ , \\ T^*G \to G \times \mathfrak{g}^*, \qquad & (g, p) \mapsto (g, (T_e^* L_g)p) = (g, \mu) \ , \end{aligned}$$

where $\mathfrak{g}$ and $\mathfrak{g}^*$ are the Lie algebra of G and its dual, and e denotes the identity element of G. Equivalent results can be obtained using right translation.

Our next topic will be the equations of motion resulting from this process.

3.3.1 Lagrangian mechanics. Euler-Poincaré equations

We could work exactly as we did in section 3.1.1 by simply prescribing that our configuration manifold is a Lie group G [CMO14; Ise+00b], but the problem becomes more interesting when we consider the possibility of left or right trivialization (we will only consider the first, but computations are analogous).

Let us define the *trivialized Lagrangian* $\ell : G \times \mathfrak{g} \to \mathbb{R}$, by $\ell(g, \eta) = L(g, T_e L_g \eta)$. Observe that the quotient of the tangent bundle by the group is $TG/G \cong \mathfrak{g}$. If the Lagrangian is completely G-invariant, i.e. for all $g' \in G$ and $(g, v) \in TG$, $L(g, v) = L(g'g, T_g L_{g'} v)$, then we can define a *reduced Lagrangian*, which we will denote with the same symbol, $\ell : \mathfrak{g} \to \mathbb{R}$, by $\ell(\eta) = L(e, T_e L_g \eta)$ [MR99].

We will work first in the trivialized setting, because the results are more general than in the reduced case, and moving to the reduced case will be a matter of eliminating a term.

In order to obtain the equations of motion it is common to consider an action of the form

$$\mathcal{J}[c] = \int_{t_a}^{t_b} \ell(g(t), \eta(t)) \mathrm{d}t$$

with $c(t) = (g(t), \eta(t)) \in G \times \mathfrak{g}$. Proceeding like this is necessary to prescribe variations of the form

$$\delta\eta = \dot{\zeta} + \mathrm{ad}_\eta \zeta, \tag{3.15}$$

with $\zeta \in \mathfrak{g}$, such that $\delta\eta(t_a) = \delta\eta(t_b) = 0$.

Instead, we will use the Hamilton-Pontryagin principle we saw in section 3.1.3 to obtain the equations of motion in a very straightforward manner. Both methods are equivalent and this way those variations appear naturally from the manipulation of the principle.

Let us rewrite the integrand in eq.(3.7) applying left-trivialization:

$$\ell(g(t), \eta(t)) + \left\langle \mu(t), T_{g(t)} L_{g^{-1}(t)} \dot{g}(t) - \eta(t) \right\rangle \tag{3.16}$$

with $\mu(t) \in \mathfrak{g}^*$ as defined in the beginning of the section.

In order to generate a variational principle it is natural to consider the space of curves

$$\begin{aligned} & C^1((g_a, \eta_a, \mu_a), (g_b, \eta_b, \mu_b), [t_a, t_b]) \\ & = \big\{ (g, \eta, \mu) : [t_a, t_b] \to G \times \mathfrak{g} \times \mathfrak{g}^* \,|\, g \in C^2([t_a, t_b]), \eta, \mu \in C^1([t_a, t_b]), \\ & \quad (g, \eta, \mu)(t_a) = (g_a, \eta_a, \mu_a), (g, \eta, \mu)(t_b) = (g_b, \eta_b, \mu_b) \big\} \, , \end{aligned}$$

and define the trivialized functional $\mathcal{J}_{\mathcal{HP}} : C^1((g_a, \eta_a, \mu_a), (g_b, \eta_b, \mu_b), [t_a, t_b]) \to \mathbb{R}$:

$$\mathcal{J}_{\mathcal{HP}}[(g, \eta, \mu)] = \int_{t_a}^{t_b} \left[\ell(g(t), \eta(t)) + \left\langle \mu(t), T_{g(t)}L_{g^{-1}(t)}\dot{g}(t) - \eta(t)\right\rangle\right] \mathrm{d}t. \tag{3.17}$$

Note that $G \times \mathfrak{g} \times \mathfrak{g}^*$ is the trivialization of $\mathbb{T}G$, as would be expected.

Let us take a family of curves $(g_\epsilon(t), \eta_\epsilon(t), \mu_\epsilon(t))$ with $\epsilon \in \mathbb{R}$ such that $(g_0(t), \eta_0(t), \mu_0(t))$ $= (g(t), \eta(t), \mu(t))$ with variations

$$\begin{aligned}
\delta g(t) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} g_\epsilon(t)\bigg|_{\epsilon=0}, \\
\delta \eta(t) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} \eta_\epsilon(t)\bigg|_{\epsilon=0}, \\
\delta \mu(t) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} \mu_\epsilon(t)\bigg|_{\epsilon=0},
\end{aligned}$$

and define the curve $\zeta(t) \in \mathfrak{g}$ by

$$\delta g(t) = T_e L_{g(t)} \zeta(t).$$

Taking into account that

$$\dot{g}_\epsilon(t) = T_e L_{g_\epsilon(t)} \eta_\epsilon(t)$$

it is not difficult to show that eq.(3.15) holds for this ζ. Using this we can easily compute the variation of $\mathcal{J}_{\mathcal{HP}}[(g, \eta, \mu)]$,

$$\mathrm{d}\mathcal{J}_{\mathcal{HP}}[(g, \eta, \mu)]((\delta g, \delta\eta, \delta\mu)) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} \mathcal{J}_{\mathcal{HP}}[(g_\epsilon, \eta_\epsilon, \mu_\epsilon)]\bigg|_{\epsilon=0}$$

This then tells us that for the extended curve (g, η, μ) to be an admissible critical point of the action the following equations must be satisfied:

$$\begin{aligned}
\frac{\mathrm{d}\mu(t)}{\mathrm{d}t} &= \mathrm{ad}^*_{\eta(t)}\mu(t) + \left(L_{g(t)}\right)^* D_1\ell(g(t), \eta(t)), \\
\mu(t) &= D_2\ell(g(t), \eta(t)), \\
\frac{\mathrm{d}g(t)}{\mathrm{d}t} &= T_e L_{g(t)}\eta(t), \quad \forall t \in [t_a, t_b].
\end{aligned}$$

These are the corresponding **trivialized Euler-Lagrange equations** of the problem, and again this is telling us that the trivialized multipliers μ coincide with the trivialized canonical momenta on $\mathfrak{g}^*$. Inserting the second equation into the first we may cast these equations in the standard form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta}\right) - \mathrm{ad}^*_{\eta(t)}\left(\frac{\partial \ell}{\partial \eta}\right) = L^*_{g(t)}\frac{\partial \ell}{\partial g}$$

In the trivialized case the third equation is coupled with this one by its right hand side, telling us exactly how to relate the group element g with the algebra element η.

If variations are taken without imposing fixed end-point conditions we obtain the boundary terms:

$$\langle \mu(t), \zeta(t)\rangle\big|_{t_a}^{t_b} = \langle \mu(t_b), \zeta(t_b)\rangle - \langle \mu(t_a), \zeta(t_a)\rangle \tag{3.18}$$

where $\zeta(t) = T_{g(t)}L_{g^{-1}(t)}\delta g(t)$.

If the Lagrangian is G-invariant, then the reduced Euler-Lagrange equations are called **Euler-Poincaré equations** and they become

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta}\right) - \mathrm{ad}^*_{\eta(t)}\left(\frac{\partial \ell}{\partial \eta}\right) = 0\,.$$

In this case, the third equation, which can be written in a more compact manner as

$$\dot{g} = g\eta,$$

is completely decoupled from the rest. In the context of reduction theory this equation is known as the **reconstruction equation** allowing us to move from the quotient back to TG. To find a solution $t \mapsto g(t)$ to the Euler-Lagrange equations, with initial condition $g(0) = g_0$ and $\dot{g}(0) = v_0$, we first solve the first order differential equation defined by the Euler-Poincaré equations with initial condition $\eta(0) = g_0^{-1}v_0$ and with this solution $t \to \eta(t)$ we solve the reconstruction equation.

If we fix a basis $\{e_a\}$ of the Lie algebra $\mathfrak{g}$, inducing coordinates (η^a) such that $\eta = \eta^a e_a$, then the Euler-Poincaré equations have the following expression in local coordinates

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta^a}\right) = C^d_{ba}\eta^b\frac{\partial \ell}{\partial \eta^d}$$

where C^d_{ab} are the structure constants of the Lie algebra $\mathfrak{g}$.

We can define a fibre derivative $\mathbb{F}\ell : G \times \mathfrak{g} \to G \times \mathfrak{g}^*$ as we did in the standard case, by

$$\langle \mathbb{F}\ell(g,\eta), \zeta\rangle = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \ell(g, \eta + t\zeta),$$

where $\eta, \zeta \in \mathfrak{g}$, which in coordinates can be expressed as

$$\mathbb{F}\ell(g,\eta) = \left(g^i, \frac{\partial \ell}{\partial \eta^i}(g,\eta)\right).$$

Clearly, this map is related with $\mathbb{F}L$ by

$$(T^*_e L_g)\mathbb{F}L(g, (T_e L_g)\eta) = \mathbb{F}\ell(g,\eta)\,.$$

We say that ℓ is regular if its fibre derivative is a local diffeomorphism. With it we can define the associated energy function as

$$E_\ell(g,\eta) = \left\langle \frac{\partial \ell}{\partial \eta}, \eta \right\rangle - \ell(g,\eta)\,.$$

Obviously, all of this holds in the reduced case.

3.3.2 Hamiltonian mechanics. Lie-Poisson equations

Let us define the *trivialized Hamiltonian* $\hbar : G \times \mathfrak{g}^* \to \mathbb{R}$, by $\hbar(g,\mu) = H(g, (T^*_g L_{g^{-1}})\mu)$. The quotient of the cotangent bundle by the group is $T^*G/G \cong \mathfrak{g}^*$. If the Hamiltonian is completely G-invariant, i.e. for $\forall k \in G$ and $(g,p) \in T^*G$, $H(g,p) = H(kg, T^*_{kg}L_{k^{-1}}p)$, then we can define a *reduced Hamiltonian*, which we will denote with the same symbol, $\hbar : \mathfrak{g}^* \to \mathbb{R}$, by $\hbar(\mu) = H(e, T^*_e L_{g^{-1}}\mu)$ [MR99; Mar18].

The most convenient way to find the Hamilton equations of motion in the trivialized case is to look back at the Lagrangian side. If $\ell : G \times \mathfrak{g} \to \mathbb{R}$ is a regular trivialized Lagrangian, then we can define an implicit trivialized Hamiltonian by $\hbar \circ \mathbb{F}\ell = E_\ell$. Using this and the equations obtained from the Hamilton-Pontryagin principle, it is not difficult to see that the Hamiltonian equations must be

$$\dot{g} = (L_g)_* \frac{\partial \hbar}{\partial \mu}\,,$$
$$\dot{\mu} = \mathrm{ad}^*_{\frac{\partial \hbar}{\partial \mu}} \mu - (L_g)^* \frac{\partial}{\partial g} \hbar(g, \mu)\,.$$

In the G-invariant case, with $\hbar' \equiv \frac{\partial \hbar}{\partial \mu}$, these equations reduce to

$$\dot{\mu} = \mathrm{ad}^*_{\hbar'(\mu)} \mu\,, \tag{3.19}$$
$$\dot{g} = g\hbar'(\mu)\,. \tag{3.20}$$

These are called the **Lie-Poisson equations**.

The manifold $G \times \mathfrak{g}^*$ still has a symplectic structure as it is isomorphic to T^*G, which is itself a symplectic manifold with symplectic form ω_G, but $\mathfrak{g}^*$ will not be symplectic in general (the dimensions do not match the requirements if $\dim \mathfrak{g}^*$ odd). Yet $\mathfrak{g}^*$ is naturally equipped with a Lie-Poisson bracket $\{\ ,\ \}$

$$\{f, g\} = -\left\langle \mu, \left[\frac{\partial f}{\partial \mu}, \frac{\partial g}{\partial \mu}\right]\right\rangle$$

where $f, g \in C^\infty(\mathfrak{g}^*)$ [see MR99, theorem 13.1.1].

In coordinates μ_a, induced by the dual basis $\{e^a\}$ on $\mathfrak{g}^*$, we have that

$$\{\mu_a, \mu_b\} = -C^d_{ab}\mu_d\,.$$

This means that $(\mathfrak{g}^*, \{\ ,\ \})$ is a Poisson manifold. In fact, this bracket exactly corresponds to the reduced bracket by standard Poisson reduction from $\pi : (T^*G, \omega_G) \to (T^*G/G \equiv \mathfrak{g}^*, \{\ ,\ \})$ where $\pi(\mu_g) = [\mu_g] \equiv T^*_e L_g(\mu_g)$.

If we fix $\mu_0 \in \mathfrak{g}^*$, we say the set

$$\mathcal{O}_{\mu_0} = \left\{\mathrm{Ad}^*_{g^{-1}}\mu_0 \mid g \in G\right\} \subseteq \mathfrak{g}^*$$

is its **coadjoint orbit**. If $t \to \mu(t)$ is the solution of the initial value problem $\dot{\mu} = \mathrm{ad}^*_{\hbar'(\mu)}\mu$ with $\mu(0) = \mu_0$, then we can deduce that $\mu(t) \in \mathcal{O}_{\mu(0)}$.

Given a Hamiltonian function $\hbar : \mathfrak{g}^* \to \mathbb{R}$ we could also derive the equations of motion by

$$\dot{\mu}(t) = \sharp^\Pi(\mathrm{d}\hbar(\mu(t))) \tag{3.21}$$

where Π is the bivector field associated to the bracket $\{\ ,\ \}$. It is well known that the flow $F^t_\hbar : \mathfrak{g}^* \to \mathfrak{g}^*$ of $X_\hbar$ verifies some geometric properties:

1. It preserves the linear Poisson bracket, that is
$$\left\{f \circ F^t_\hbar, g \circ F^t_\hbar\right\} = \{f, g\} \circ F^t_\hbar, \quad \forall f, g \in C^\infty(\mathfrak{g}^*).$$
2. It preserves the Hamiltonian $\hbar \circ F^t_\hbar = \hbar$.
3. If all the coadjoint orbits are connected, Casimir functions are also preserved along each coadjoint orbit.

3.4 Discrete mechanics on Lie groups

By far the most common way to tackle the Lie group case in discrete mechanics is to work as we have done before [CMO14; Ise+00b], and apply reduction afterwards. Therefore, we define a discrete Lagrangian on our group G, $L_d : G \times G \to \mathbb{R}$, and a discrete curve as a map $c_d : T_d \to G$, with $T_d = \{t_i\}_{i=0}^N \in \mathbb{R}$. Again, we will assume we are working with constant time-step curves, $t_{i+1} - t_i = h, \forall i = 0, ..., N-1$, with $h \in \mathbb{R}$. All the essential curve spaces remain the same and our discrete action is now

$$\begin{array}{rccl} \mathcal{J}_d : & C_d\left(g_a, g_b\right) & \longrightarrow & \mathbb{R} \\ & c_d & \longmapsto & \sum_{k=0}^{N-1} L_d(g_k, g_{k+1}), \end{array}$$

with $g_a = g_0$ and $g_b = g_N$.

Direct application of the discrete Hamilton's principle leads to the usual discrete Euler-Lagrange equations

$$D_2 L_d(g_{i-1}, g_i) + D_1 L_d(g_i, g_{i+1}) = 0, \quad i = 1, ..., N-1\,.$$

Now assume this discrete Lagrangian is G-invariant, i.e. it satisfies that $\forall g' \in G$, $L_d(g'g_k, g'g_{k+1}) = L_d(g_k, g_{k+1})$. Then we can define a discrete (left-)reduced Lagrangian, $\ell : G \to \mathbb{R}$ by

$$\ell_d(g_k^{-1} g_{k+1}) = L_d(e, g_k^{-1} g_{k+1})\,.$$

This is tantamount to taking the quotient $(G \times G)/G \cong G$, with quotient map $\pi_G^{\text{red}} : G \times G \to (G \times G)/G$, $(g_k, g_{k+1}) \mapsto (g_k^{-1} g_{k+1})$ [see MPS99]. If we define $W_k = g_k^{-1} g_{k+1}$, then the discrete action can be rewritten as

$$\mathcal{J}_d[c_d] = \sum_{k=0}^{N-1} \ell_d(W_k)\,.$$

Similar to the continuous case, we can impose variations ζ_k of the form

$$\delta W_k = -\zeta_k W_k + W_k \zeta_{k+1}, \quad \text{for } k = 0, ..., N-1\,.$$

The form of these variations is easy to understand by identifying $\zeta_k = g_k^{-1} \delta g_k$.

With these, the resulting discrete Euler-Poincaré equations can be written as

$$L^*_{W_k} \ell'_d(W_k) - R^*_{W_{k+1}} \ell'_d(W_{k+1}) = 0, \quad \text{for } k = 0, ...N-1\,,$$

or, more commonly, either

$$L^*_{W_{k+1}} \ell'_d(W_{k+1}) = \mathrm{Ad}^*_{W_{k+1}} \left(L^*_{W_k} \ell'_d(W_k)\right)$$

or

$$R^*_{W_{k+1}} \ell'_d(W_{k+1}) = \mathrm{Ad}^*_{W_k} \left(R^*_{W_k} \ell'_d(W_k)\right)\,.$$

The first version can be also rewritten as

$$\overleftarrow{\xi}_{W_k}(\ell_d) - \overrightarrow{\xi}_{W_{k+1}}(\ell_d) = 0\,, \quad \forall \xi \in \mathfrak{g}\,.$$

Here $\overleftarrow{\xi}_W = T_e L_W \xi$ and $\overrightarrow{\xi}_W = T_e R_W \xi$ are the left and right-invariant vector fields associated with ξ, respectively. This version remains valid even in the Lie groupoid setting [see MMM06].

3.4.1 Intrinsic discrete Lagrangian formalism

Alternatively, we can obtain the discrete Euler-Poincaré equations *intrinsically*, that is, without mention of any pre-existing non-reduced Lagrangian [see MMM06, for more details].

Given a fixed element $W \in G$, define the set of admissible pairs

$$C_W^2 = \{(W_1, W_2) \in G \times G \,|\, W_1 W_2 = W\}\,.$$

A tangent vector to the manifold C_W^2 is a tangent vector at $t = 0$ of a curve in C_W^2

$$t \in (-\epsilon, \epsilon) \subseteq \mathbb{R} \to (c_1(t), c_2(t))$$

where $c_i(t) \in G$, $c_1(t)c_2(t) = W$ and $c_1(0) = W_1$ and $c_2(0) = W_2$. These types of curve are given by

$$c(t) = (W_1 U(t), U^{-1}(t) W_2) \tag{3.22}$$

for an arbitrary $U(t) \in G$ with $t \in (-\epsilon, \epsilon)$ and $U(0) = e$, where e is the identity element of G.

Given a discrete Lagrangian $\ell_d : G \to \mathbb{R}$, we define the **discrete action functional** by

$$\begin{array}{rccc} \mathcal{J}_d : & C_W^2 & \to & \mathbb{R} \\ & (W_1, W_2) & \mapsto & \ell_d(W_1) + \ell_d(W_2)\,. \end{array}$$

Definition 3.4.1. (**Discrete Hamilton's principle on Lie groups**) Given $W \in G$, then $(W_1, W_2) \in C_W^2$ is a solution of the discrete Lagrangian system determined by $\ell_d : G \to \mathbb{R}$ if and only if (W_1, W_2) is a critical point of $\mathcal{J}_d$.

We characterize the critical points using the curves defined in (3.22) as follows

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{J}_d[c(t)]\Big|_{t=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}t} \left[\ell_d(W_1 U(t)) + \ell_d(U(t)^{-1} W_2)\right]\Big|_{t=0} \\ &= \left\langle L_{W_1}^* \mathrm{d}\ell_d - R_{W_2}^* \mathrm{d}\ell_d, \zeta \right\rangle \end{aligned}$$

where $\zeta = \dot{U}(0)$.

3.4.2 Discrete fibre derivative

First consider the maps $\mathbb{F}^{\pm} L_d : G \times G \to T^*G$ defined by

$$\begin{aligned} \mathbb{F}^- L_d(g_0, g_1) &= (g_0, p_0 = -D_1 L_d(g_0, g_1)), \\ \mathbb{F}^+ L_d(g_0, g_1) &= (g_1, p_1 = D_2 L_d(g_0, g_1)). \end{aligned}$$

Note that we can left (or right) trivialize the fibre derivative to obtain $\mathbb{F}^{\pm} L_d^{\text{left}} : G \times G \to G \times \mathfrak{g}^*$,

$$\begin{aligned} \mathbb{F}^- L_d^{\text{left}}(g_0, g_1) &= (g_0, \mu_0 = -L_{g_0}^* D_1 L_d(g_0, g_1)), \\ \mathbb{F}^+ L_d^{\text{left}}(g_0, g_1) &= (g_1, \mu_1 = L_{g_1}^* D_2 L_d(g_0, g_1)). \end{aligned}$$

Identifying terms in the equality

$$\left\langle -R^*_{g_0^{-1}g_1}\ell'_d(g_0^{-1}g_1), \zeta_0 \right\rangle + \left\langle L^*_{g_0^{-1}g_1}\ell'_d(g_0^{-1}g_1), \zeta_1 \right\rangle = \left\langle L^*_{g_0} D_1 L_d(g_0, g_1), \zeta_0 \right\rangle + \left\langle L^*_{g_1} D_2 L_d(g_0, g_1), \zeta_1 \right\rangle$$

with $\zeta_k = g_k^{-1}\delta g_{k+1}$, leads us to finally define maps $\mathbb{F}^{\pm}\ell_d : G \to \mathfrak{g}^*$ by

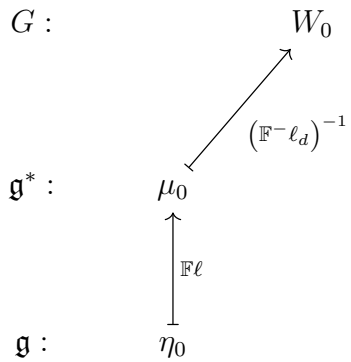
$$\mathbb{F}^-\ell_d(W) = R^*_W \ell'_d(W),$$
$$\mathbb{F}^+\ell_d(W) = L^*_W \ell'_d(W).$$

These are the **reduced discrete fibre derivatives**. We say that the discrete reduced Lagrangian is regular if both discrete fibre derivatives are local diffeomorphisms, which is equivalent to the regularity of the matrix whose coefficients are (ℓ''_d).

3.4.3 Correspondence with continuous mechanics and Lie group integrators

The theory of the exact discrete Lagrangian remains valid here, so in this setting we can also define the order of an approximation in the same way as we did before.

As in any other case, one should always be mindful of how to properly initialize any integration method. Assume we are working in the reduced case and we are given an initial condition $(g_0, \eta_0) \in G \times \mathfrak{g}$. We can check eq.(3.18) and establish that if we had the exact discrete Lagrangian at our disposal, the proper way to initialize our method would be to identify the boundary terms of the continuous and discrete case. Thus, it makes sense to apply the continuous fibre derivative to transform the initial condition η_0 to $\mu_0 = \mathbb{F}\ell(\eta_0)$ and then apply the discrete fibre derivative to obtain W_0.



Once the complete sequence $\{W_k\}_{k=0}^{N-1}$ is obtained, the reconstruction on G is then easily obtained by using the discrete reconstruction equation

$$g_{k+1} = g_k W_k \,.$$

3.4.4 Variational Lie group integrators

In order to obtain numerical integrators we need to find a way to either connect $L_d(g_k, g_{k+1})$ with $L(g(t), \eta(t))$ or connect $\ell_d(W_k)$ with $\ell(\eta)$. This can be done in several ways, either by using natural charts, applying Galerkin methods with curves on G or simply taking crude approximations as if we were working in a vector space.

As in this work we are mainly concerned with Runge-Kutta collocation methods, for us it will be convenient to go back to the Hamilton-Pontryagin setting.

Consider the action in eq.(3.17). We want to discretize this action, and in particular we need to know how to properly discretise the kinematic constraint $\dot{g}(t) = v(t) = T_e L_{g(t)}\eta(t)$. Again, we will consider RK methods for this but we must be mindful of the geometric structure of the configuration manifold.

The work of H. Munthe-Kaas [Mun99] was one of the first to tackle the problem of generalizing RK-type algorithms to more general manifolds and specifically to the Lie group case. In this work the author acknowledges the fact that one needs a vector space structure in order to apply a RK method, as they rely heavily on its linear structure. In order to address this issue, one can exploit the structure of Lie group of G and its relation with its Lie algebra $\mathfrak{g}$, which is a vector space (see section 2.3.6).

We will consider the local diffeomorphism $\tau : \mathfrak{g} \to U_e \subset G$, where U_e is a neighborhood of the identity element, as retraction maps. The most common instances of these are the exponential map, exp, and the Cayley map, cay (in the case of quadratic Lie groups).

Assuming that G is connected, we will be able to translate a neighborhood of any point to U_e and from U_e to $\mathfrak{g}$ and back thanks to τ^{-1} and τ. Not only that, but this will also be possible in $\mathbb{T}G = TG \oplus T^*G$, which is what we need for our mechanical problems.

For some $h \in G$, the complete geometric scheme is as follows:

$$\begin{array}{ccccc}
\mathbb{T}\mathfrak{g} & \underset{\mathbb{T}\tau^{-1}}{\overset{\mathbb{T}\tau}{\rightleftarrows}} & \mathbb{T}U_e & \underset{\mathbb{T}L_h^{-1}=\mathbb{T}L_{h^{-1}}}{\overset{\mathbb{T}L_h}{\rightleftarrows}} & \mathbb{T}G \\
\downarrow{\scriptstyle \pi_{\mathfrak{g}}} & & \downarrow{\scriptstyle \pi_U} & & \downarrow{\scriptstyle \pi_G} \\
\mathfrak{g} & \underset{\tau^{-1}}{\overset{\tau}{\rightleftarrows}} & U_e & \underset{L_h^{-1}=L_{h^{-1}}}{\overset{L_h}{\rightleftarrows}} & G
\end{array}$$

with

$$\mathbb{T}\tau(\xi, \eta_\xi, \mu_\xi) \;=\; (\tau(\xi), T_\xi\tau(\xi), (T_{\tau(\xi)}\tau^{-1})^*\mu_\xi)$$

where $\xi \in \mathfrak{g}$, $\eta_\xi \in T_\xi\mathfrak{g} \cong \mathfrak{g}$ and $\mu_\xi \in T^*_\xi\mathfrak{g} \cong \mathfrak{g}^*$ and similar definitions for the other maps.

Assume we work with adapted coordinates $(g, v, p) \in \mathbb{T}G$ and $(\xi, \eta_\xi, \mu_\xi) \in \mathbb{T}\mathfrak{g}$. According to this diagram, if h is such that $L_{h^{-1}}g \in U_e$, we find the following correspondences:

$$\begin{aligned}
&\mathbb{T}_{L_{h^{-1}}g}\tau^{-1}\mathbb{T}_g L_{h^{-1}}(g, v, p) \\
&\quad = \left(\tau^{-1}\left(L_{h^{-1}}g\right), \mathrm{d}^L\tau^{-1}_{\tau^{-1}(L_{h^{-1}}g)} T_g L_{g^{-1}} v, \left(\mathrm{d}^L\tau_{\tau^{-1}(L_{h^{-1}}g)}\right)^* (T_e L_g)^* p\right) \\
&\quad = (\xi, \eta_\xi, \mu_\xi) \\
&\mathbb{T}_{\tau(\xi)} L_h \mathbb{T}_\xi \tau(\xi, \eta_\xi, \mu_\xi) \\
&\quad = \left(L_h\tau(\xi), T_e L_{L_h\tau(\xi)} \mathrm{d}^L\tau_\xi \eta_\xi, \left(T_{L_h\tau(\xi)} L_{(L_h\tau(\xi))^{-1}}\right)^* \left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \mu_\xi\right) \\
&\quad = (g, v, p)
\end{aligned}$$

where $\mathrm{d}^L\tau : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ and $\mathrm{d}^L\tau^{-1} : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ were defined in section 2.3.6.

Let us also take this opportunity to define $\mathrm{dd}^L\tau : \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, the **second left-trivialised tangent**, which will be necessary for later derivations (see section 3.4.5 for a better picture). This is a linear map in the second and third variables such that $\partial_\xi \left(\mathrm{d}^L\tau_\xi \eta\right) \delta\xi = \mathrm{d}^L\tau_\xi \mathrm{dd}^L\tau_\xi(\eta, \delta\xi)$. It appears naturally when representing elements

$(g, v, a) \in T^{(2)}G$, the second order tangent bundle of G (see section 2.1.2), with elements of $(\xi, \eta, \zeta) \in T^{(2)}\mathfrak{g}$, which using matrix notation becomes:

$$\left(e, g^{-1}v, g^{-1}a - g^{-1}vg^{-1}v\right) \mapsto \left(0, \mathrm{d}^L\tau_\xi\eta, \mathrm{d}^L\tau_\xi\left[\zeta + \mathrm{dd}^L\tau_\xi(\eta,\eta)\right]\right) .$$

With this, RKMK methods for our kinematic constraint can be obtained (see section 2.3.6). Using matrix notation, our continuous constraint becomes $\dot{g}(t) = g(t)\eta(t)$, and its discrete version can be written as:

$$\tau^{-1}((g_k)^{-1}G_k^i) = h\sum_{j=1}^{s} a_{ij}\mathrm{d}^L\tau^{-1}_{\tau^{-1}((g_k)^{-1}G_k^j)}(G_k^j)^{-1}V_k^j ,$$
$$\tau^{-1}((g_k)^{-1}g_{k+1}) = h\sum_{j=1}^{s} b_j\mathrm{d}^L\tau^{-1}_{\tau^{-1}((g_k)^{-1}G_k^j)}(G_k^j)^{-1}V_k^j ,$$

which, if $V_k^i = G_k^i\mathrm{d}^L\tau_{\tau^{-1}((g_k)^{-1}G_k^i)}\mathrm{H}_k^i$ (where H is capital η), reduces to

$$\tau^{-1}((g_k)^{-1}G_k^i) = h\sum_{j=1}^{s} a_{ij}\mathrm{H}_k^j ,$$
$$\tau^{-1}((g_k)^{-1}g_{k+1}) = h\sum_{j=1}^{s} b_j\mathrm{H}_k^j .$$

With the above expressions, the discrete Hamilton-Pontryagin eq.(3.12) on a Lie group transforms into:

$$\begin{aligned}(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[& L\left(G_k^i, V_k^i\right) \\ & + \left\langle \tilde{P}_k^i, \frac{1}{h}G_k^i\tau^{-1}((g_k)^{-1}G_k^i) - G_k^i\sum_{j=1}^{s} a_{ij}\mathrm{d}^L\tau^{-1}_{\tau^{-1}((g_k)^{-1}G_k^j)}(G_k^j)^{-1}V_k^j \right\rangle \\ & + \left\langle \tilde{p}_{k+1}, \frac{1}{h}g_{k+1}\tau^{-1}((g_k)^{-1}g_{k+1}) - g_{k+1}\sum_{j=1}^{s} b_j\mathrm{d}^L\tau^{-1}_{\tau^{-1}((g_k)^{-1}G_k^j)}(G_k^j)^{-1}V_k^j \right\rangle \Bigg]\end{aligned}$$

where $\tilde{P}_k^i \in T^*_{G_k^i}G$ and $\tilde{p}_{k+1} \in T^*_{g_{k+1}}G$. We can shorten this expression to:

$$\begin{aligned}(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[& L\left(G_k^i, V_k^i\right) \\ & + \left\langle \widetilde{\mathrm{M}}_k^i, \frac{1}{h}\tau^{-1}((g_k)^{-1}G_k^i) - \sum_{j=1}^{s} a_{ij}\mathrm{d}^L\tau^{-1}_{\tau^{-1}((g_k)^{-1}G_k^j)}(G_k^j)^{-1}V_k^j \right\rangle \\ & + \left\langle \tilde{\mu}_{k+1}, \frac{1}{h}\tau^{-1}((g_k)^{-1}g_{k+1}) - \sum_{j=1}^{s} b_j\mathrm{d}^L\tau^{-1}_{\tau^{-1}((g_k)^{-1}G_k^j)}(G_k^j)^{-1}V_k^j \right\rangle \Bigg]\end{aligned}$$

where $\tilde{\mu}_k, \widetilde{\mathrm{M}}_k^i \in \mathfrak{g}^*$.

Using elements $(\Xi_k^i, \mathrm{H}_k^i) \in T\mathfrak{g}$ as representatives of $(G_k^i, V_k^j) \in TG$, we find:

$$(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} hb_i \left[L\left(g_k\tau(\Xi_k^i), g_k\tau(\Xi_k^i)\mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right) + \left\langle \widetilde{\mathrm{M}}_k^i, \frac{1}{h}\Xi_k^i - \sum_{j=1}^{s} a_{ij}\mathrm{H}_k^j \right\rangle + \left\langle \tilde{\mu}_{k+1}, \frac{1}{h}\tau^{-1}((g_k)^{-1}g_{k+1}) - \sum_{j=1}^{s} b_j\mathrm{H}_k^j \right\rangle \right].$$

Expressing the Lagrangian $L : TG \to \mathbb{R}$ as $\ell : G \times \mathfrak{g} \to \mathbb{R}$ using left translation, this expression simplifies to

$$(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} hb_i \left[\ell\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right) + \left\langle \widetilde{\mathrm{M}}_k^i, \frac{1}{h}\Xi_k^i - \sum_{j=1}^{s} a_{ij}\mathrm{H}_k^j \right\rangle + \left\langle \tilde{\mu}_{k+1}, \frac{1}{h}\tau^{-1}((g_k)^{-1}g_{k+1}) - \sum_{j=1}^{s} b_j\mathrm{H}_k^j \right\rangle \right], \tag{3.23}$$

which is the discrete equivalent of (3.17) and the one we will work with from here on.

Similarly as we did in the vector space case, let us consider the space of s-stage *variationally partitioned Runge-Kutta-Munthe-Kaas* sequences (*s-stage VPRKMK sequences*):

$$C_d^s(g_a, g_b) = \left\{ \left(g, \tilde{\mu}, \left\{\Xi^i, \mathrm{H}^i, \widetilde{\mathrm{M}}^i\right\}_{i=1}^{s}\right) : \{t_k\}_{k=0}^{N} \to G \times \mathfrak{g}^* \times (\mathbb{T}\mathfrak{g})^s \mid g(a) = g_a, g(b) = g_b \right\}.$$

Note that $\mathbb{T}\mathfrak{g} \cong \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g}^*$.

Now we are in a position to state the Lie group analogue of theorem 3.2.4. This will be a more general version of [BM09, theorem 4.9], which is order 2-bound. In fact ours is essentially equivalent to the approach in [BM16, section 4.1], but without resorting to any truncation.

Theorem 3.4.1. *Let $\ell : G \times \mathfrak{g} \to \mathbb{R}$ be a C^l function with $l \geq 2$ and an s-stage VPRKMK sequence $c_d \in C_d^s(g_0, g_N)$. Then c_d is a critical point of the discrete Hamilton-Pontryagin functional, $(\mathcal{J}_{\mathcal{HP}})_d$, if and only if for all $k = 0, ..., N-1$ and $i = 1, ..., s$ it satisfies*

$$\Xi_k^i = \tau^{-1}\left(g_k^{-1}G_k^i\right) = h\sum_{j=1}^{s} a_{ij}\mathrm{H}_k^j, \tag{3.24}$$

$$\xi_{k,k+1} = \tau^{-1}\left(g_k^{-1}g_{k+1}\right) = h\sum_{j=1}^{s} b_j\mathrm{H}_k^j, \tag{3.25}$$

$$\mathrm{M}_k^i = \mathrm{Ad}^*_{\tau(\xi_{k,k+1})}\left[\mu_k + h\sum_{j=1}^{s} b_j\left(\mathrm{d}^L\tau^{-1}_{-\Xi_k^j} - \frac{a_{ji}}{b_i}\mathrm{d}^L\tau^{-1}_{-\xi_{k,k+1}}\right)^* \mathrm{N}_k^j\right], \tag{3.26}$$

$$\mu_{k+1} = \mathrm{Ad}^*_{\tau(\xi_{k,k+1})}\left[\mu_k + h\sum_{j=1}^{s} b_j\left(\mathrm{d}^L\tau^{-1}_{-\Xi_k^j}\right)^* \mathrm{N}_k^j\right]; \tag{3.27}$$

where

$$\begin{aligned}
\mathrm{N}_k^i &= \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{g_k\tau(\Xi_k^i)} D_1\ell\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right),\\
\mathrm{M}_k^i &= \left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^* \left[\Pi_k^i + h\sum_{j=1}^s \frac{b_j a_{ji}}{b_i}\left(\mathrm{dd}^L\tau_{\Xi_k^j}\right)^*\left(\mathrm{H}_k^j, \Pi_k^j\right)\right],\\
\Pi_k^i &= \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* D_2\ell\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right),\\
\mu_k &= \left(\mathrm{d}^L\tau^{-1}_{\xi_{k-1,k}}\right)^*\tilde{\mu}_k.
\end{aligned}$$

Proof. We know that c_d is a critical point of the discrete Hamilton-Pontryagin functional if and only if $\mathrm{d}\left(\mathcal{J}_{\mathcal{HP}}\right)_d(c_d)(\delta c_d) = 0$, $\forall \delta c_d \in T_{c_d}C_d^s(g_0, g_N)$. Let us write $\delta c_d = \left(\delta g, \delta\tilde{\mu}, \left\{\delta\Xi^i, \delta\mathrm{H}^i, \delta\widetilde{\mathrm{M}}^i\right\}_{i=1}^s\right)$ and compute each of the individual variations separated from each other:

$$\begin{aligned}
\delta g : \sum_{k=0}^{N-1}\sum_{i=1}^s hb_i \Bigg[&\left\langle D_1\ell\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right), \delta g_k\tau(\Xi_k^i)\right\rangle\\
&+ \left\langle \tilde{\mu}_{k+1}, \frac{1}{h}D\tau^{-1}((g_k)^{-1}g_{k+1})(-(g_k)^{-1}\delta g_k(g_k)^{-1}g_{k+1} + (g_k)^{-1}\delta g_{k+1})\right\rangle\Bigg].
\end{aligned}$$

As it is customary we will define new variations $\zeta_k = (g_k)^{-1}\delta g_k \in \mathfrak{g}$ and use these to rewrite this equation, together with the trivialised tangents and the short-hand $\xi_{k,k+1} = \tau^{-1}((g_k)^{-1}g_{k+1})$:

$$\begin{aligned}
\delta g : \sum_{k=0}^{N-1}\sum_{i=1}^s hb_i \Bigg[&\left\langle D_1\ell\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right), g_k\tau(\Xi_k^i)\tau(-\Xi_k^i)\zeta_k\tau(\Xi_k^i)\right\rangle\\
&+ \left\langle \tilde{\mu}_{k+1}, \frac{1}{h}\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}(-\mathrm{Ad}^{-1}_{\tau\left(\xi_{k,k+1}\right)}\zeta_k + \zeta_{k+1})\right\rangle\Bigg]\\
= \sum_{k=0}^{N-1}\Bigg[&\left\langle h\sum_{i=1}^s b_i\left(\mathrm{Ad}^{-1}_{\tau(\Xi_k^i)}\right)^* L^*_{g_k\tau(\Xi_k^i)} D_1\ell\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right), \zeta_k\right\rangle\\
&- \left\langle\left(\mathrm{Ad}^{-1}_{\tau\left(\xi_{k,k+1}\right)}\right)^*\left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^*\tilde{\mu}_{k+1}, \zeta_k\right\rangle\\
&+ \left\langle\left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^*\tilde{\mu}_{k+1}, \zeta_{k+1}\right\rangle\Bigg]
\end{aligned}$$

where we have used the order one condition. If we rearrange the sum so that terms with the same ζ_k appear together (the discrete analogue of integration by parts) we are left

with:

$$\begin{aligned}\delta g : \sum_{k=1}^{N-1} \Bigg[\Bigg\langle & h \sum_{i=1}^{s} b_i \left(\mathrm{Ad}^{-1}_{\tau(\Xi^i_k)}\right)^* L^*_{g_k\tau(\Xi^i_k)} D_1\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right) \\ & - \left(\mathrm{Ad}^{-1}_{\tau\left(\xi_{k,k+1}\right)}\right)^* \left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^* \tilde{\mu}_{k+1} + \left(\mathrm{d}^L\tau^{-1}_{\xi_{k-1,k}}\right)^* \tilde{\mu}_k, \zeta_k \Bigg\rangle \Bigg] \\ & + \Bigg\langle h \sum_{i=1}^{s} b_i \left(\mathrm{Ad}^{-1}_{\tau(\Xi^i_k)}\right)^* L^*_{g_k\tau(\Xi^i_k)} D_1\ell \left(g_0\tau(\Xi^i_0), \mathrm{d}^L\tau_{\Xi^i_0}\mathrm{H}^i_0\right) \\ & - \left(\mathrm{Ad}^{-1}_{\tau(\Xi_{0,1})}\right)^* \left(\mathrm{d}^L\tau^{-1}_{\Xi_{0,1}}\right)^* \tilde{\mu}_1, \zeta_0 \Bigg\rangle + \left\langle \left(\mathrm{d}^L\tau^{-1}_{\Xi_{N-1,N}}\right)^* \tilde{\mu}_N, \zeta_N \right\rangle .\end{aligned}$$

Identification of the boundary terms with their counterparts on the continuous realm suggests the change $\left(\mathrm{d}^L\tau^{-1}_{\xi_{k-1,k}}\right)^* \tilde{\mu}_k = \mu_k$.

Let us move on to a different variation:

$$\begin{aligned}\delta\Xi : \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[& \left\langle D_1\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), g_k D\tau(\Xi^i_k)\delta\Xi^i_k \right\rangle \\ & + \left\langle D_2\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), \partial_{\Xi^i_k}\left(\mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right)\delta\Xi^i_k \right\rangle + \left\langle \frac{1}{h}\widetilde{\mathrm{M}}^i_k, \delta\Xi^i_k \right\rangle \Bigg] .\end{aligned}$$

Using the definition of $\mathrm{dd}^L\tau$ we can rewrite this as:

$$\begin{aligned}\delta\Xi : & \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[\left\langle D_1\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), g_k\tau(\Xi^i_k)\mathrm{d}^L\tau_{\Xi^i_k}\delta\Xi^i_k \right\rangle \\ & + \left\langle D_2\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{dd}^L\tau_{\Xi^i_k}(\mathrm{H}^i_k, \delta\Xi^i_k) \right\rangle + \left\langle \widetilde{\mathrm{M}}^i_k, \frac{1}{h}\delta\Xi^i_k \right\rangle \Bigg] \\ & = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[\left\langle \left(\mathrm{d}^L\tau_{\Xi^i_k}\right)^* L^*_{g_k\tau(\Xi^i_k)} D_1\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), \delta\Xi^i_k \right\rangle \\ & + \left\langle \left(\mathrm{dd}^L\tau_{\Xi^i_k}\right)^* \left(\mathrm{H}^i_k, \left(\mathrm{d}^L\tau_{\Xi^i_k}\right)^* D_2\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right)\right) + \frac{1}{h}\widetilde{\mathrm{M}}^i_k, \delta\Xi^i_k \right\rangle \Bigg] .\end{aligned}$$

It is now the turn of variations with respect to $\delta\mathrm{H}$:

$$\begin{aligned}\delta\mathrm{H} : \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[& \left\langle D_2\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), \mathrm{d}^L\tau_{\Xi^i_k}\delta\mathrm{H}^i_k \right\rangle \\ & - \left\langle \widetilde{\mathrm{M}}^i_k, \sum_{j=1}^{s} a_{ij}\delta\mathrm{H}^j_k \right\rangle - \left\langle \tilde{\mu}_{k+1}, \sum_{j=1}^{s} b_j\delta\mathrm{H}^j_k \right\rangle \Bigg] \\ & = \sum_{k=0}^{N-1}\sum_{i=1}^{s} h \Bigg[\left\langle b_i \left(\mathrm{d}^L\tau_{\Xi^i_k}\right)^* D_2\ell \left(g_k\tau(\Xi^i_k), \mathrm{d}^L\tau_{\Xi^i_k}\mathrm{H}^i_k\right), \delta\mathrm{H}^i_k \right\rangle \\ & - \left\langle \sum_{j=1}^{s} b_j a_{ji}\widetilde{\mathrm{M}}^j_k, \delta\mathrm{H}^i_k \right\rangle - \left\langle b_i\tilde{\mu}_{k+1}, \delta\mathrm{H}^i_k \right\rangle \Bigg]\end{aligned}$$

where we have used the order 1 condition again and we have also rearranged summation indices.

The last two variations are the easiest ones, as they are nothing but the RKMK constraints:

$$\delta\widetilde{\mathrm{M}}, \delta\tilde{\mu} : \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left[\left\langle \delta\widetilde{\mathrm{M}}_k^i, \frac{1}{h}\Xi_k^i - \sum_{j=1}^{s} a_{ij}\mathrm{H}_k^j \right\rangle + \left\langle \delta\tilde{\mu}_{k+1}, \frac{1}{h}\tau^{-1}((g_k)^{-1}g_{k+1}) - \sum_{j=1}^{s} b_j \mathrm{H}_k^j \right\rangle \right].$$

After imposing fixed-end variations we are left with the following set of equations for $k = 1, ..., N-1$ and $i = 1, ..., s$:

$$\mu_{k+1} = \mathrm{Ad}^*_{\tau(\xi_{k,k+1})} \left[\mu_k + h\sum_{i=1}^{s} b_i \left(\mathrm{Ad}^{-1}_{\tau(\Xi_k^i)}\right)^* L^*_{g_k\tau(\Xi_k^i)} D_1\ell \left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i \right) \right], \tag{3.28}$$

$$\begin{aligned} \widetilde{\mathrm{M}}_k^i = -h \Big[&\left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{g_k\tau(\Xi_k^i)} D_1\ell \left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i \right) \\ &+ \left(\mathrm{dd}^L\tau_{\Xi_k^i}\right)^* \left(\mathrm{H}_k^i, \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* D_2\ell \left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i \right) \right) \Big], \end{aligned} \tag{3.29}$$

$$\left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* D_2\ell \left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i \right) - \sum_{j=1}^{s} \frac{b_j a_{ji}}{b_i}\widetilde{\mathrm{M}}_k^j - \left(\mathrm{d}^L\tau_{\xi_{k,k+1}}\right)^* \mu_{k+1} = 0, \tag{3.30}$$

$$\Xi_k^i = h\sum_{j=1}^{s} a_{ij}\mathrm{H}_k^j, \tag{3.31}$$

$$\xi_{k,k+1} = h\sum_{j=1}^{s} b_j \mathrm{H}_k^j. \tag{3.32}$$

Using some of the shorthand variables defined in the statement of the theorem we may rewrite eqs.(3.28) and (3.29) as

$$\begin{aligned} \mu_{k+1} &= \mathrm{Ad}^*_{\tau(\xi_{k,k+1})} \left[\mu_k + h\sum_{j=1}^{s} b_j \left(\mathrm{d}^L\tau^{-1}_{-\Xi_k^j}\right)^* \mathrm{N}_k^j \right], \\ \widetilde{\mathrm{M}}_k^i &= -h \left[\mathrm{N}_k^i + \left(\mathrm{dd}^L\tau_{\Xi_k^i}\right)^* \left(\mathrm{H}_k^i, \Pi_k^i\right) \right], \end{aligned}$$

where in the first one we have also used the fact that $\mathrm{d}^L\tau_{\Xi}^{-1}\mathrm{Ad}^{-1}_{\tau(\Xi)} = \mathrm{d}^L\tau^{-1}_{-\Xi}$. This first one is in fact one of the equations we were after.

Inserting both of these in eq.(3.30), and leaving only terms with Π_k on the left-hand side we finally obtain:

$$\mathrm{M}_k^i = \mathrm{Ad}^*_{\tau(\xi_{k,k+1})} \left[\mu_k + h\sum_{j=1}^{s} b_j \left(\mathrm{d}^L\tau^{-1}_{-\Xi_k^j} - \frac{a_{ji}}{b_i}\mathrm{d}^L\tau^{-1}_{-\xi_{k,k+1}} \right)^* \mathrm{N}_k^j \right]$$

which is the remaining equation we wanted to obtain. □

Remark. It is worth noting that perhaps eq.(3.26) is not the most geometric way to express such a relation. That form has been chosen for notational economy and mnemotechnic reasons.

In order to give a more geometrically sound version of this equation we should identify the different elements that appear in it. First, let us consider a point $(G_k^i, V_k^i) \in TG$ and the section of T^*TG induced by $\mathrm{d}L$ on that point, i.e.

$$\left(G_k^i, V_k^i, D_1L(G_k^i, V_k^i), D_2L(G_k^i, V_k^i)\right) \in T^*TG.$$

One may rush to the conclusion that if we represent such an element in $T^*T\mathfrak{g}$ we should get:

$$\begin{aligned}\Big(\Xi_k^i, \mathrm{H}_k^i, \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{L_{g_k}\tau\left(\Xi_k^i\right)} D_1L(L_{g_k}\tau\left(\Xi_k^i\right), (L_{g_k})_*\,\mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i),\\ \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{L_{g_k}\tau\left(\Xi_k^i\right)} D_2L(L_{g_k}\tau\left(\Xi_k^i\right), (L_{g_k})_*\,\mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i)\Big),\end{aligned}$$

which, using the invariance of the Lagrangian, reduces to

$$\begin{aligned}\Big(\Xi_k^i, \mathrm{H}_k^i, \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{L_{g_k}\tau\left(\Xi_k^i\right)} D_1\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i),\\ \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* D_2\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i)\Big),\end{aligned}$$

but this is not correct in this instance. The reason for this is that this expression is not compatible with the restriction of the natural pairing $\langle\cdot,\cdot\rangle : TTG \times T^*TG \to \mathbb{R}$ to $T^{(2)}G$ (see section 3.4.6). This compatibility is required to obtain the correct invariance when considering Tulczyjew's triple (see sections 2.1.2 and 3.1.5), which allows us to interpret the third component as the "*velocity*" associated with the canonical momenta. In particular, $\alpha_G^{-1} : T^*TG \to TT^*G$, $(g, v, P_q, P_v) \mapsto (g, p = P_v, V_g = v, V_p = P_q)$.

Thus, the correct representation in $T^*T\mathfrak{g}$ must be:

$$\begin{aligned}\Big(\Xi_k^i, \mathrm{H}_k^i, \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{L_{g_k}\tau\left(\Xi_k^i\right)} D_1\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i)\\ + \left(\mathrm{dd}^L\tau_{\Xi_k^i}\right)^* \left(\Xi_k^i, \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* D_2\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i)\right),\\ \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* D_2\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i)\Big).\end{aligned}$$

Clearly, $\widetilde{\mathrm{M}}_k^i$ is proportional to this third component. If we transport this element from Ξ_k^i to $0 \in \mathfrak{g}$ we are left with:

$$\left(0, \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i, L^*_{L_{g_k}\tau\left(\Xi_k^i\right)} D_1\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i), D_2\ell(L_{g_k}\tau\left(\Xi_k^i\right), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i)\right)$$

which shows that this third component becomes $\left(\mathrm{d}^L\tau^{-1}_{\Xi_k^i}\right)^* \mathrm{N}_k^i$.

In order to simplify the final expression, let us write these as $\left(\xi_k^i, \eta_{\xi_k}^i, \nu_{\xi_k}^i, \mu_{\xi_k}^i\right)$ and $(0, \eta_0^i, \nu_0^i, \mu_0^i)$ respectively. Taking this into account we can finally rewrite eq.(3.26) as

$$\begin{aligned}&\left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^* \mu_{\xi_k}^i =\\ &\mathrm{Ad}^*_{\tau(\xi_{k,k+1})}\left\{\mu_k + h\sum_{j=1}^s b_j\left[\left(\mathrm{Ad}^{-1}_{\tau(\xi_k^j)}\right)^* \nu_0^j - \frac{a_{ji}}{b_i}\left(\mathrm{Ad}^{-1}_{\tau(\xi_{k,k+1})}\right)^* \left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^* \nu_{\xi_k}^j\right]\right\},\end{aligned}$$

and if we use the notation $\left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^* \zeta_{\xi}{}^i_k = \hat{\zeta}_{\xi}{}^i_k$, this reduces to

$$\hat{\mu}_{\xi}{}^i_k = \mathrm{Ad}^*_{\tau(\xi_{k,k+1})}\left\{\mu_k + h\sum_{j=1}^{s} b_j\left[\left(\mathrm{Ad}^{-1}_{\tau(\xi^j_k)}\right)^*\nu_0^j - \frac{a_{ji}}{b_i}\left(\mathrm{Ad}^{-1}_{\tau(\xi_{k,k+1})}\right)^*\hat{\nu}_{\xi}{}^j_k\right]\right\}. \qquad \triangle$$

3.4.5 Some relations of the second trivialized tangent

For the sake of completeness we offer the following section to complete the picture of the map $\mathrm{dd}^L\tau$.

To make geometric sense of this operator consider $T\mathrm{d}^L\tau$, the tangent to the map $\mathrm{d}^L\tau : T\mathfrak{g} \to T\mathfrak{g}, (\xi,\eta) \mapsto (0, \mathrm{d}^L\tau_\xi\eta)$. From this we see that $\mathrm{d}^L\tau$ is effectively acting as a translation operator on $T\mathfrak{g}$. $\mathrm{dd}^L\tau$ can then be seen as a double bundle extension of this tangent operator:

$$\begin{array}{rccc} T\mathrm{d}^L\tau : & TT\mathfrak{g} & \to & TT\mathfrak{g} \\ & (\xi,\eta,V_\xi,V_\eta) & \mapsto & \left(0, \mathrm{d}^L\tau_\xi\eta, \mathrm{d}^L\tau_\xi V_\xi, \mathrm{d}^L\tau_\xi\left(\mathrm{dd}^L\tau_\xi(\eta,V_\xi)+V_\eta\right)\right). \end{array}$$

When restricted to $T^{(2)}\mathfrak{g}$, that is, when $V_\xi = \eta$, we get

$$\begin{array}{rccc} T\mathrm{d}^L\tau\big|_{T^{(2)}\mathfrak{g}} : & T^{(2)}\mathfrak{g} & \to & T^{(2)}\mathfrak{g} \\ & (\xi,\eta,\zeta) & \mapsto & \left(0, \mathrm{d}^L\tau_\xi\eta, \mathrm{d}^L\tau_\xi\left(\zeta+\mathrm{dd}^L\tau_\xi(\eta,\eta)\right)\right). \end{array}$$

In what follows we will derive several identities related to this operator.

Lemma 3.4.2. *The tangent of the inverse tangent of τ satisfies*

$$\partial_\xi\left(\mathrm{d}^L\tau_\xi^{-1}\eta\right)\zeta = -\mathrm{dd}^L\tau_\xi\left(\mathrm{d}^L\tau_\xi^{-1}\eta,\zeta\right)$$

for $(\xi,\eta,\zeta) \in T^{(2)}\mathfrak{g}$.

Proof. First, consider the identity

$$\mathrm{d}^L\tau_\xi\mathrm{d}^L\tau_\xi^{-1}\eta = \eta\,.$$

If we differentiate on both sides we get

$$\partial_\xi\left(\mathrm{d}^L\tau_\xi\mathrm{d}^L\tau_\xi^{-1}\eta\right)\zeta = 0\,,$$

and expanding the left-hand side

$$\begin{aligned}\partial_\xi\left(\mathrm{d}^L\tau_\xi\mathrm{d}^L\tau_\xi^{-1}\eta\right)\zeta &= \partial_{\hat{\xi}}\left(\mathrm{d}^L\tau_{\hat{\xi}}\mathrm{d}^L\tau_\xi^{-1}\eta\right)\zeta\Big|_{\hat{\xi}=\xi} + \mathrm{d}^L\tau_\xi\partial_\xi\left(\mathrm{d}^L\tau_\xi^{-1}\eta\right)\zeta \\ &= \mathrm{d}^L\tau_\xi\mathrm{dd}^L\tau_\xi\left(\mathrm{d}^L\tau_\xi^{-1}\eta,\zeta\right) + \mathrm{d}^L\tau_\xi\partial_\xi\left(\mathrm{d}^L\tau_\xi^{-1}\eta\right)\zeta\,.\end{aligned}$$

From here we can extract the result we were looking for. □

Lemma 3.4.3. *For any $(\xi,\eta,\zeta) \in T^{(2)}\mathfrak{g}$, the following identity holds*

$$\mathrm{dd}^L\tau_\xi(\eta,\zeta) + \mathrm{dd}^L\tau_{-\xi}(\eta,\zeta) = \mathrm{d}^L\tau_{-\xi}^{-1}\mathrm{ad}_{\mathrm{d}^L\tau_\xi\zeta}\mathrm{d}^L\tau_{-\xi}\eta\,.$$

Proof. Consider the identity

$$\mathrm{d}^L\tau_\xi\eta = \mathrm{Ad}_{\tau(\xi)}\mathrm{d}^L\tau_{-\xi}\eta \tag{3.33}$$

consequence of lemma 2.3.5.

If we differentiate on both sides we get

$$\begin{aligned}\partial_\xi\left(\mathrm{d}^L\tau_\xi\eta\right)\zeta &= \partial_\xi\left(\mathrm{Ad}_{\tau(\xi)}\mathrm{d}^L\tau_{-\xi}\eta\right)\zeta \\ &= \partial_{\hat\xi}\left(\mathrm{Ad}_{\tau(\hat\xi)}\mathrm{d}^L\tau_{-\xi}\eta\right)\zeta\Big|_{\hat\xi=\xi} + \mathrm{Ad}_{\tau(\xi)}\partial_\xi\left(\mathrm{d}^L\tau_{-\xi}\eta\right)\zeta\,.\end{aligned}$$

Let us deal with the first term on the right-hand size. For this we need to differentiate the Ad operator:

$$\begin{aligned}\partial_\xi\left(\mathrm{Ad}_{\tau(\xi)}\eta\right)\zeta &= \partial_\xi\left(\tau(\xi)\eta\left(\tau(\xi)\right)^{-1}\right)\zeta \\ &= D\tau(\xi)\zeta\eta\left(\tau(\xi)\right)^{-1} - \tau(\xi)\eta\left(\tau(\xi)\right)^{-1}D\tau(\xi)\zeta\left(\tau(\xi)\right)^{-1} \\ &= \mathrm{Ad}_{\tau(\xi)}\left(\left(\tau(\xi)\right)^{-1}D\tau(\xi)\zeta\eta - \eta\left(\tau(\xi)\right)^{-1}D\tau(\xi)\zeta\right) \\ &= \mathrm{Ad}_{\tau(\xi)}\left(\mathrm{d}^L\tau_\xi\zeta\eta - \eta\mathrm{d}^L\tau_\xi\zeta\right) \\ &= \mathrm{Ad}_{\tau(\xi)}\mathrm{ad}_{\mathrm{d}^L\tau_\xi\zeta}\eta\,.\end{aligned}$$

For the second term we need only the following identity

$$\partial_\xi\left(\mathrm{d}^L\tau_{-\xi}\eta\right)\zeta = -\mathrm{d}^L\tau_{-\xi}\mathrm{dd}^L\tau_{-\xi}\left(\eta,\zeta\right)\,.$$

These, together with eq.(3.33), lead to

$$\mathrm{d}^L\tau_\xi\mathrm{dd}^L\tau_\xi\left(\eta,\zeta\right) = \mathrm{Ad}_{\tau(\xi)}\mathrm{ad}_{\mathrm{d}^L\tau_\xi\zeta}\mathrm{d}^L\tau_{-\xi}\eta - \mathrm{d}^L\tau_\xi\mathrm{dd}^L\tau_{-\xi}\left(\eta,\zeta\right)\,, \tag{3.34}$$

which after regrouping leads to the identity we were after. □

Finally, we offer here a simple relation that can be easily obtained from eq.(2.30) for the exponential

$$\mathrm{dd}^L\exp_0(\eta,\zeta) = -\frac{1}{2}\mathrm{ad}_\eta\zeta\,, \qquad \mathrm{dd}^R\exp_0(\eta,\zeta) = \frac{1}{2}\mathrm{ad}_\eta\zeta\,.$$

3.4.6 The second trivialized tangent and $T^*T\mathfrak{g}$

Remember that if $g \in U_e$, then we may represent $(g,v,a) \in T^{(2)}G$ by an element of $(\xi,\eta,\zeta) \in T^{(2)}\mathfrak{g}$ via left-trivialization as

$$\left(\tau(\xi), \tau(\xi)\mathrm{d}^L\tau_\xi\eta, \tau(\xi)\left\{\left(\mathrm{d}^L\tau_\xi\eta\right)\left(\mathrm{d}^L\tau_\xi\eta\right) + \mathrm{d}^L\tau_\xi\left[\zeta + \mathrm{dd}^L\tau_\xi\left(\eta,\eta\right)\right]\right\}\right)\,.$$

We may left-translate this to the zero element of $\mathfrak{g}$ and obtain a point

$$(0,\eta_0,\zeta_0) = \left(0, \mathrm{d}^L\tau_\xi\eta, \mathrm{d}^L\tau_\xi\left[\zeta + \mathrm{dd}^L\tau_\xi\left(\eta,\eta\right)\right]\right) \in T^{(2)}\mathfrak{g}\,.$$

Now, let $(\xi,\eta,\nu,\mu)\,,(0,\eta_0,\nu_0,\mu_0) \in T^*T\mathfrak{g}$ denote two points such that one is obtained by left translation of the other. Let us find a transformation rule that relates these two such that it is compatible with the structure just presented in $T^{(2)}\mathfrak{g}$. To do so, we may apply the pairing $\langle\cdot,\cdot\rangle : TT\mathfrak{g}\times T^*T\mathfrak{g} \to \mathbb{R}$ and impose:

$$\langle(\nu_0,\mu_0)\,,(V_{\xi_0},V_{\eta_0})\rangle = \langle(\nu,\mu)\,,(V_\xi,V_\eta)\rangle\,,$$

and later restrict to $T^{(2)}\mathfrak{g}$, that is, $(V_{\xi_0}, V_{\eta_0}) = (\eta_0, \zeta_0)$.

By expanding the left-hand side of the previous equality we get

$$\begin{aligned}
\langle (\nu,\mu), (V_\xi, V_\eta)\rangle &= \left\langle (\nu_0,\mu_0), \left(\mathrm{d}^L\tau_\xi V_\xi, \mathrm{d}^L\tau_\xi \left[V_\eta + \mathrm{dd}^L\tau_\xi(\eta, V_\xi)\right]\right)\right\rangle \\
&= \left\langle \nu_0, \mathrm{d}^L\tau_\xi V_\xi\right\rangle + \left\langle \mu_0, \mathrm{d}^L\tau_\xi\left[V_\eta + \mathrm{dd}^L\tau_\xi(\eta, V_\xi)\right]\right\rangle \\
&= \left\langle \left(\mathrm{d}^L\tau_\xi\right)^* \nu_0, V_\xi\right\rangle + \left\langle \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0, V_\eta + \mathrm{dd}^L\tau_\xi(\eta, V_\xi)\right\rangle \\
&= \left\langle \left(\mathrm{d}^L\tau_\xi\right)^* \nu_0, V_\xi\right\rangle + \left\langle \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0, V_\eta\right\rangle \\
&\quad + \left\langle \left(\mathrm{dd}^L\tau_\xi\right)^* \left(\eta, \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0\right), V_\xi\right\rangle \\
&= \left\langle \left(\left(\mathrm{d}^L\tau_\xi\right)^* \nu_0 + \left(\mathrm{dd}^L\tau_\xi\right)^* \left(\eta, \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0\right), \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0\right), (V_\xi, V_\eta)\right\rangle
\end{aligned}$$

and after restricting this to $T^{(2)}\mathfrak{g}$ we obtain:

$$\begin{aligned}
\nu &= \left(\mathrm{d}^L\tau_\xi\right)^* \nu_0 + \left(\mathrm{dd}^L\tau_\xi\right)^* \left(\eta, \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0\right), & \nu_0 &= \left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \left[\nu - \left(\mathrm{dd}^L\tau_\xi\right)^* (\eta,\mu)\right], \\
\mu &= \left(\mathrm{d}^L\tau_\xi\right)^* \mu_0 & \mu_0 &= \left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \mu
\end{aligned}$$

.

This in turn leads to a relation between $(g, v, P_g, P_v) \in T^*TG$ and (ξ, η, ν, μ):

$$\begin{aligned}
(g, v, P_g, P_v) = \big(&\tau(\xi), \tau(\xi)\mathrm{d}^L\tau_\xi\eta, \\
&(\tau(-\xi))^* \left\{\left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \left[\nu - \left(\mathrm{dd}^L\tau_\xi\right)^* (\eta,\mu)\right] - \left(\mathrm{d}^L\tau_\xi\eta\right)^* \left(\left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \mu\right)\right\}, \\
&(\tau(-\xi))^* \left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \mu\big) \ .
\end{aligned}$$

Chapter 4

Variational error analysis for forced mechanical systems

4.1 Introduction to forced mechanical systems

By forced systems we refer to systems under the influence of forcing which cannot be absorbed into the Lagrangian or Hamiltonian as part of a potential [see Lán70; GPS02]. As we will see in a moment, such systems do not admit a traditional variational description without additional considerations; therefore, they present a problem when proving the order of forced variational integrators.

In the later part of this chapter we will devote ourselves to the study of a novel technique to transform forced problems into purely variational ones, allowing us to apply the result of theorem 3.2.2 after discretizing the resulting variational principle.

4.1.1 Lagrangian description

A Lagrangian *external force* is usually defined as a map $f^L : TQ \to T^*Q$ such that $\pi_Q \circ f^L = \tau_Q$ [see BC99; MW01], that is

$$\begin{array}{ccc} TQ & \xrightarrow{\quad f^L \quad} & T^*Q \\ & {\scriptstyle \tau_Q} \searrow \quad \swarrow {\scriptstyle \pi_Q} & \\ & Q & \end{array}$$

In adapted local coordinates they take the form

$$f^L(q, v) = (q^i, f_i^L(q, v)) \,.$$

Let us define the **virtual work** done by a given force as the functional

$$\mathcal{W}^f[c](X) = \int_{t_a}^{t_b} \left\langle f^L(\hat{c}(t)), X(t) \right\rangle \mathrm{d}t$$

where $c \in C^2(q_a, q_b, [t_a, t_b])$ and $X \in T_c C^2(q_a, q_b, [t_a, t_b])$. The term *virtual* comes from the fact that an arbitrary X can be interpreted as a virtual motion of the system and the classical concept of work was reserved for the case where $X(t) = \hat{c}(t)$, where the latter is

the tangent lift of c. In this sense, the variation of our action functional can be regarded as a virtual work too, called *virtual work due to the inertial forces*,

$$\mathcal{W}^I[c](X) = \mathrm{d}\mathcal{J}[c](X).$$

The total virtual work of a system is then

$$\mathcal{W}^T[c](X) = \mathcal{W}^I[c](X) + \mathcal{W}^f[c](X)$$

which if $X = \frac{\mathrm{d}}{\mathrm{d}\epsilon} c_\epsilon(t)\big|_{\epsilon=0}$ we can write as

$$\mathcal{W}^T[c](X) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} \int_{t_a}^{t_b} L(\hat{c}_\epsilon(t))\mathrm{d}t \,\Big|_{\epsilon=0} + \int_{t_a}^{t_b} \left\langle f^L(\hat{c}(t)), \frac{\mathrm{d}}{\mathrm{d}\epsilon} c_\epsilon(t)\Big|_{\epsilon=0} \right\rangle \mathrm{d}t\,.$$

The Lagrange-D'Alembert principle is a physical principle that tells us how to find physical trajectories in the presence of external forces, where Hamilton's principle cannot help us.

Definition 4.1.1. (Lagrange-D'Alembert principle). A curve $c \in C^2(q_a, q_b, [t_a, t_b])$ is the *physical trajectory* of the forced Lagrangian system defined by the Lagrangian $L : TQ \to \mathbb{R}$ and the external force $f^L : TQ \to T^*Q$ if and only if $\mathcal{W}^T[c](\delta c) = 0$ for all $\delta c \in T_c C^2(q_a, q_b, [t_a, t_b])$.

In local coordinates the resulting equations given by the principle take the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = f_i^L(q(t), \dot{q}(t)) \tag{4.1}$$

which we may also write as

$$D_{\mathrm{EL}} L(\hat{c}^{(2)}(t)) = f^L(\hat{c}(t)).$$

We will call them **forced Euler-Lagrange equations**.

Given an external force we can construct a semibasic 1-form $\mu_L \in \Omega^1(TQ)$ by the relation

$$\langle \mu_L(v_q), X_{v_q} \rangle = \langle f^L(v_q), T\tau_Q(X_{v_q}) \rangle, \quad \forall X_{v_q} \in T_{v_q} TQ\,.$$

In coordinates, this takes the form

$$\mu_L = f_i^L(q^i, v^i)\, \mathrm{d}q^i\,.$$

With this semibasic forcing form, the forced Euler-Lagrange equations can be recast into a more geometric form as

$$\imath_{X^f_{E_L}} \omega_L = \mathrm{d}E_L - \mu_L\,,$$

which is of the same form as eq.(3.3). Here the integral curves of the vector field $X^f_{E_L}$ are the solutions to the forced Euler-Lagrange equations.

Due to the linearity of this equation the vector field $X^f_{E_L}$ can be decomposed into two parts as $X_{E_L} + Z^v_f$. X_{E_L} is the Hamiltonian part of the vector field, i.e. the one in eq.(3.3), and $Z^v_f \in VTQ \subset TTQ$ is the part due to the forcing

$$\imath_{Z^v_f} \omega_L = -\mu_L\,.$$

In local coordinates this last vector field can be written as

$$Z^v_f = (g_L)^{ij} f^L_j \partial_{v^i}\,.$$

Lagrangian forcing in Lie groups

Assuming our configuration manifold is a Lie group G with Lie algebra $\mathfrak{g}$, a Lagrangian external force $f^L : TG \to T^*G$ can be trivialized as the Lagrangian itself. We define the trivialized force as a map $f^\ell : G \times \mathfrak{g} \to G \times \mathfrak{g}^*$ by the relation

$$f^\ell(g, \eta) = (T_e^* L_g) f^L(g, (T_e L_g)\eta)\,.$$

Noting that the forcing always enters the Euler-Lagrange equations as the potential terms, that is, as the partial derivatives with respect to the base coordinates, it is easy to guess the correct form of the trivialized forced equations:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta}\right) - \mathrm{ad}^*_{\eta(t)}\left(\frac{\partial \ell}{\partial \eta}\right) &= L^*_{g(t)}\left(\frac{\partial \ell}{\partial g} + f^L(g(t), (L_{g(t)})_*\eta(t))\right) \\ &= L^*_{g(t)}\frac{\partial \ell}{\partial g} + f^\ell(g(t), \eta(t)).\end{aligned}$$

In the reduced setting an external force is a map $f^\ell : \mathfrak{g} \to \mathfrak{g}^*$, where we are purposefully overloading the same symbol as in the trivialized case. The forced Euler-Poincaré equations then take the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta}\right) - \mathrm{ad}^*_{\eta(t)}\left(\frac{\partial \ell}{\partial \eta}\right) = f^\ell(\eta(t))\,.$$

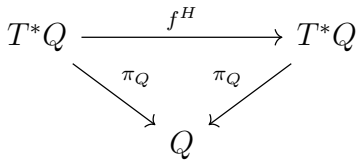
Given a basis $\{e_a\}$ of $\mathfrak{g}$, and inducing coordinates (η^a) such that $\eta = \eta^a e_a$, then the forced Euler-Poincaré equations have the following expression in local coordinates

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta^a}\right) = C^d_{ba}\eta^b \frac{\partial \ell}{\partial \eta^d} + f^\ell_a\,,$$

where $\left\langle f^\ell(\eta), e_a \right\rangle = f^\ell_a$.

4.1.2 Hamiltonian description

In analogy to the Lagrangian case, we can say that a Hamiltonian *external force* is defined by a map $f^H : T^*Q \to T^*Q$ such that $\pi_Q \circ f^H = \pi_Q$, that is



In adapted local coordinates they take the form

$$f^H(q, p) = (q^i, f^H_i(q, p))\,.$$

Still, perhaps the most natural way to think about a Hamiltonian force is as a semibasic form $\mu_H \in \Omega^1(T^*Q)$. With it the forced Hamilton equations can be written as

$$\imath_{X^f_H}\omega_Q = \mathrm{d}H - \mu_H$$

which in coordinates becomes

$$\dot{q}^i = \frac{\partial H}{\partial p_i}(q,p)\,,$$
$$\dot{p}_i = -\frac{\partial H}{\partial q^i}(q,p) + f_i^H(q,p)\,.$$

Again, the field can be decomposed as $X_H^f = X_H + Y_H^v$, where the latter, $Y_f^v \in VT^*Q \subset TT^*Q$, can be defined as the vertical lift

$$Y_f^v(\alpha_q) = \frac{\mathrm{d}}{\mathrm{d}t}(\alpha_q + t f^H(\alpha_q))\bigg|_{t=0}\,.$$

Locally this is,

$$Y_f^v = f_i^H(q,p)\partial_{p_i}\,.$$

Given a Lagrangian external force and a Hamiltonian, we may define a Hamiltonian external force based on the former as $f^H = \mathbb{F}H^* f^L$, which in coordinates is

$$f^H(q,p) = \left(q^i, f_i^L\left(q, \frac{\partial H}{\partial p}(q,p)\right)\right)\,.$$

Hamiltonian forcing in Lie groups

A Hamiltonian external force on a Lie group can be trivialized into a map $f^\hbar : G \times \mathfrak{g}^* \to G \times \mathfrak{g}^*$ defined by the relation

$$f^\hbar(g,\mu) = (T_e^* L_g) f^H(g, (T_g^* L_{g^{-1}})\mu)\,.$$

The trivialized Hamilton equations of motion are

$$\dot{g} = (L_g)_* \frac{\partial \hbar}{\partial \mu}\,,$$
$$\dot{\mu} = \mathrm{ad}^*_{\frac{\partial \hbar}{\partial \mu}}\mu - (L_g)^* \frac{\partial \hbar}{\partial g} + f^\hbar(g,\mu)\,.$$

In the reduced setting, a force becomes a map $f^\hbar : \mathfrak{g}^* \to \mathfrak{g}^*$, and the Lie-Poisson equations of motion are then

$$\dot{\mu} = \mathrm{ad}^*_{\frac{\partial \hbar}{\partial \mu}}\mu + f^\hbar(\mu)\,.$$

Starting from a reduced Lagrangian force $f^\ell : \mathfrak{g} \to \mathfrak{g}^*$ we can also construct a reduced Hamiltonian force via the fibre derivative $f^\hbar = f^\ell \circ \mathbb{F}\hbar$, where $\mathbb{F}\hbar : \mathfrak{g}^* \to \mathfrak{g}$ is the fibre derivative defined by $\hbar$. If $\hbar$ is derived from a regular reduced Lagrangian ℓ, then $\mathbb{F}\hbar = \mathbb{F}\ell^{-1}$, and the forced Euler-Poincaré and forced Lie-Poisson equations are equivalent.

4.2 Discrete forced mechanics and error analysis

Discrete forced mechanics revolves around the discrete version of the Lagrange-D'Alembert principle. Remember that in the continuous setting we consider total virtual work

$$\begin{aligned}\mathcal{W}^T[c](\delta c) &= \mathcal{W}^I[c](\delta c) + \mathcal{W}^f[c](\delta c)\\ &= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\int_{t_a}^{t_b} L(\hat{c}_\epsilon(t))\mathrm{d}t\,\bigg|_{\epsilon=0} + \int_{t_a}^{t_b}\left\langle f^L(\hat{c}(t)), \frac{\mathrm{d}}{\mathrm{d}\epsilon}c_\epsilon(t)\bigg|_{\epsilon=0}\right\rangle \mathrm{d}t\end{aligned}$$

where $c = c_0(t)$ and $\delta c = \frac{\mathrm{d}}{\mathrm{d}t} c_\epsilon(t)$. The first term, $\mathcal{W}^I[c](\delta c) = \mathrm{d}\mathcal{J}[c](\delta c)$, is of the same form as the varied action of the Hamilton principle, although of course, the trajectory c will not be a critical point of $\mathcal{J}[c]$ in general. As we know, the discrete counterpart of this first term is

$$\begin{aligned}\mathcal{W}_d^I[c_d](\delta c_d) = \mathrm{d}\mathcal{J}_d[c_d](\delta c_d) &= \delta\left(\sum_{k=0}^{N-1} L_d(q_k, q_{k+1})\right) \\ &= \sum_{k=0}^{N-1} \left[D_1 L_d(q_k, q_{k+1})\delta q_k + D_2 L_d(q_k, q_{k+1})\delta q_{k+1}\right].\end{aligned}$$

This causes us to propose a discrete total virtual work of the form

$$\begin{aligned}&\mathcal{W}_d^T[c_d](\delta c_d) = \mathcal{W}_d^I[c_d](\delta c_d) + \mathcal{W}_d^f[c_d](\delta c_d) \\ &= \delta\left(\sum_{k=0}^{N-1} L_d(q_k, q_{k+1})\right) + \sum_{k=0}^{N-1}\left[f_d^-(q_k, q_{k+1})\delta q_k + f_d^+(q_k, q_{k+1})\delta q_{k+1}\right] \\ &= \sum_{k=0}^{N-1}\left[\left(D_1 L_d(q_k, q_{k+1}) + f_d^-(q_k, q_{k+1})\right)\delta q_k + \left(D_2 L_d(q_k, q_{k+1}) + f_d^+(q_k, q_{k+1})\right)\delta q_{k+1}\right].\end{aligned}$$

This leads to the definition of a discrete Lagrangian force as a pair of maps $f_d^\pm : Q \times Q \to T^*Q$ such that $\pi_Q \circ f_d^- = \mathrm{pr}_1$ and $\pi_Q \circ f_d^+ = \mathrm{pr}_2$. In local coordinates these take the form

$$\begin{aligned}f_d^-(q_0, q_1) &= (q_0^i, f_{d,i}^-(q_0, q_1)), \quad \text{for } i = 1, ..., n \\ f_d^+(q_0, q_1) &= (q_1^i, f_{d,i}^+(q_0, q_1)).\end{aligned}$$

Then, the discrete Lagrange-D'Alembert principle can be stated as follows:

Definition 4.2.1. (Discrete Lagrange-D'Alembert principle). A curve $c_d \in C_d(q_a, q_b, T_d)$ is the (discrete) physical trajectory of the discrete forced Lagrangian system defined by the Lagrangian $L_d : Q \times Q \to \mathbb{R}$ and the external forcing $f_d^\pm : Q \times Q \to T^*Q$ if and only if $\mathcal{W}_d^T[c_d](\delta c_d) = 0$ for all $\delta c_d \in T_{c_d} C_d(q_a, q_b, T_d)$.

The resulting discrete forced Euler-Lagrange equations are then

$$D_2 L_d(q_{k-1}, q_k) + f_d^+(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) + f_d^-(q_k, q_{k+1}) = 0$$

which generates a discrete forced Lagrangian map (flow) $F_{L_d^f} : Q \times Q \to Q \times Q$, $(q_{i-1}, q_i) \mapsto (q_i, q_{i+1})$.

Remember that the discrete Euler-Lagrange equations can be interpreted as a matching of momenta via the fibre derivative. Analogously, we can define a pair of discrete forced fibre derivatives $\mathbb{F}^{f\pm} L_d : Q \times Q \to T^*Q$ by

$$\begin{aligned}\mathbb{F}^{f-} L_d(q_0, q_1) &= (q_0, p_0 = -D_1 L_d(q_0, q_1) - f_d^-(q_0, q_1)), \\ \mathbb{F}^{f+} L_d(q_0, q_1) &= (q_1, p_1 = D_2 L_d(q_0, q_1) + f_d^+(q_0, q_1)).\end{aligned}$$

Consequently, the discrete forced Hamiltonian map is $\widetilde{F}_{L_d^f} = \mathbb{F}^{f\pm} L_d \circ F_{L_d^f} \circ \left(\mathbb{F}^{f\pm} L_d\right)^{-1}$.

If we want to model a discrete forced Lagrangian system after a given continuous one, (Q, L, f^L), then it seems natural to define a new exact discrete Lagrangian and exact discrete forces as

$$\begin{aligned} L_d^e(q_0, q_1) &= \int_0^h L(\hat{c}(t))\mathrm{d}t\,, \\ f_d^{e-}(q_0, q_1) &= \int_0^h \left\langle f^L(\hat{c}(t)), \frac{\partial c(t)}{\partial q_0} \right\rangle \mathrm{d}t\,, \\ f_d^{e+}(q_0, q_1) &= \int_0^h \left\langle f^L(\hat{c}(t)), \frac{\partial c(t)}{\partial q_1} \right\rangle \mathrm{d}t\,, \end{aligned}$$

where now $c \in C^k\left(q_0, q_1, [0, h]\right)$, $k \geq 2$, is the solution of the forced Euler-Lagrange equations, eq.(4.1).

In [MW01], the authors state that their variational error analysis theorem can be extended to this more general case. But note that forces enter at the level of the discrete fibre derivatives. In [PC09] the authors dispute the fact that the order of the discrete fibre derivative is the same as that of the discrete flow. This casts some shadows over the validity of extending the original result to the forced case. Still, numerical experiments back the fact that forced integrators obtained by the discrete Lagrange-D'Alembert principle have the correct order.

This was one of the motivations to begin studying forced systems in a different way. What if one could completely sidestep the necessity of entering at the level of the discrete fibre derivatives? What if we could reformulate the forced problem as a free Lagrangian one (a variational one)?

4.2.1 Fokker effective actions and Galley's idea

The last question is one many physicists and mathematicians have wondered about for a long time, at least for the last century [see Bat31; FT77; MF53, for instance]. One of the main motivators for this has been the need to incorporate dissipation phenomena in the variational setting for its application in quantum mechanical problems.

The first law of thermodynamics states that the internal (i.e. total) energy of a closed (isolated) system is constant. Therefore, dissipation can only occur in an open system. Dissipation can be understood as a net flow of energy from the open system towards its environment, to which it is coupled. If the open system and its environment form a bigger closed system, its total energy must be conserved.

A classical toy model for dissipation in mechanics is precisely an arbitrary mechanical system, A, coupled to an array of harmonic oscillators, B, modelling what is known as a *bath*. The energy of A can flow towards B and back. As the number of oscillators in B goes to infinity, the time it takes for the energy absorbed by B to move back to A also goes to infinity (consequence of the Poincaré recurrence theorem). If we only consider A, it experiments a clear process of dissipation.

An important contribution to the problem of including dissipation in a variational principle, and the one we study here, is the one by C. Galley [Gal13; GTS14]. In order to motivate his idea he proposes a very simplified version of the toy model: Assume a mechanical system consisting of two harmonic oscillators of masses m and M and natural frequencies ω and Ω coupled together with coupling constant λ. This can be modeled as a Lagrangian mechanical system $(Q = \mathbb{R}^2, L)$, with $(q, Q, v, V) \in TQ$ and

$$L(q, Q, v, V) = L_{(m,\omega)}(q, v) + L_{(M,\Omega)}(Q, V) + L_\lambda(q, Q),$$

where

$$L_{(m,\omega)}(q,v) = \frac{m}{2}\left(v^2 - \omega^2 q^2\right),$$
$$L_{(M,\Omega)}(Q,V) = \frac{M}{2}\left(V^2 - \Omega^2 Q^2\right),$$
$$L_\lambda(q,Q) = \lambda q Q.$$

The Euler-Lagrange equations of motion are then

$$\ddot{q}(t) = -\omega^2 q(t) + \frac{\lambda}{m} Q(t),$$
$$\ddot{Q}(t) = -\Omega^2 Q(t) + \frac{\lambda}{M} q(t).$$

We may think about one of the oscillators as the arbitrary system we are interested in, and the second oscillator as its environment. The process known as "*integrating out*" (or integrating away) in the physics community, consists of removing part of a system and substituting it with its formal solution, so that only the subsystem under consideration is featured in the description. This is equivalent to us focusing only on system A.

In the toy system, assume we want to focus on the subsystem formed by the oscillator (m,ω) with variables $(q,v) \in T\mathbb{R}$. Integrating out the other oscillator (M,Ω) implies solving its equations of motion and substituting them in the firsts.

The solution of the second oscillator is of the form $Q(t) = Q_0(t) + Q_\lambda(t)$, where $Q_0(t)$ is the *homogeneous* solution of the problem, i.e. of

$$\ddot{Q}(t) + \Omega^2 Q(t) = 0$$

and $Q_\lambda(t)$ is the inhomogeneous solution

$$Q_\lambda(t) = \frac{\lambda}{M}\int_{t_0}^{t} G(t,s) q(s) \mathrm{d}s$$

where $G(t,s)$ is the Green function of the problem, satisfying the equation

$$\frac{\partial^2}{\partial t^2} G(t,s) + \Omega^2 G(t,s) = \delta(t-s),$$

and $\delta(x)$ is the Dirac delta distribution. For instance, given initial conditions $Q_0(0) = Q_0$ and $\dot{Q}_0(0) = V_0$ the homogeneous solution is

$$Q_0(t) = \cos(\Omega t) Q_0 + \sin(\Omega t)\frac{V_0}{\Omega}.$$

The Green function is obtained for homogeneous initial conditions $G(0,s) = 0$ and $\frac{\partial}{\partial t} G(t,s)\big|_{t=0} = 0$ resulting in

$$G(t,s) = \frac{\theta(t-s)\sin(\Omega(t-s))}{\Omega},$$

where $\theta(x)$ is the Heaviside distribution.

If we do this sort of substitution directly in the action, the resulting type of action is called a **Fokker effective action**

$$\mathcal{J}^{\text{eff}}[(q(t))] = \int_{t_a}^{t_b} \left[\frac{m}{2}\left(\dot{q}(t)^2 - \omega^2 q(t)^2\right) + \lambda q(t)\left(\widetilde{Q}_0(t) + \widetilde{Q}_\lambda(t)\right)\right] \mathrm{d}t = \int_{t_a}^{t_b} \left[\frac{m}{2}\left(\dot{q}(t)^2 - \omega^2 q(t)^2\right) + \lambda q(t)\widetilde{Q}_0(t) + \frac{\lambda^2}{M}\int_{t_a}^{t_b} q(t)\widetilde{G}(t,s)q(s)\mathrm{d}s\right] \mathrm{d}t\,.$$

Note that the integral

$$\int_{t_a}^{t_b}\int_{t_a}^{t_b} q(t)\widetilde{G}(t,s)q(s)\mathrm{d}s\mathrm{d}t$$

is symmetric, so if we apply Hamilton's principle the resulting equation of motion is

$$\ddot{q}(t) = -\omega^2 q(t) + \lambda\widetilde{Q}_0(t) + \frac{\lambda^2}{M}\int_{t_a}^{t_b}\left[\widetilde{G}(t,s) + \widetilde{G}(s,t)\right] q(s)\mathrm{d}s$$

where the symmetrized version of $\widetilde{G}(t,s)$ is coupled to q. The symmetry of the kernel implies that it can only take into account reversible or conservative interactions between the two oscillators.

$\widetilde{G}(t,s)$ is in fact a function of $t-s$ that we will denote by $\widetilde{G}_{\text{ret}}(t-s)$, called the *retarded Green function* of the problem, so the symmetric kernel inside the equation can be rewritten as

$$\widetilde{G}_{\text{ret}}(t-s) + \widetilde{G}_{\text{adv}}(t-s)$$

where $\widetilde{G}_{\text{adv}}(t-s) = \widetilde{G}_{\text{ret}}(s-t)$ is the *advanced Green function*. This implies that the evolution of the (m,ω) oscillator depends not only on its past but on its future evolution, so it is not causal.

Where did the problem come from? Galley points out that Hamilton's principle is to blame for posing a time boundary value problem instead of an initial value one, which led us to our oscillator only coupling to the symmetric part of $\widetilde{G}(t,s)$.

The solution he found is to explicitly break the time symmetry by introducing two instead of one set of variables, $q \dashrightarrow q_1, q_2$. The idea is to have a curve $q_1(t)$ advancing in time towards the end-time boundary and the other curve $q_2(t)$ advancing backwards in time satisfying that $q_1(t_b) = q_2(t_b)$ and $\dot{q}_1(t_b) = \dot{q}_2(t_b)$ (see fig. 4.1). This way we can write the action as

$$\begin{aligned}\mathcal{J}_0[(q_1(t), q_2(t))] &= \int_{t_a}^{t_b} L(q_1(t), \dot{q}_1(t))\mathrm{d}t + \int_{t_b}^{t_a} L(q_2(t), \dot{q}_2(t))\mathrm{d}t \\ &= \int_{t_a}^{t_b} \left[L(q_1(t), \dot{q}_1(t)) - L(q_2(t), \dot{q}_2(t))\right] \mathrm{d}t\,.\end{aligned}$$

Note that the actual value of $q_i(t_b)$, $i = 1, 2$, is not set. The only values that are set are the initial ones, namely $q_1(t_a) = q_{1,a}$ and $q_2(t_a) = q_{2,a}$.

An action of this type opens the door to adding more general terms, such as a coupling function $K(q_1, q_2, v_1, v_2)$ so that we get a new action

$$\mathcal{J}_K[(q_1(t), q_2(t))] = \int_{t_a}^{t_b} \left[L(q_1(t), \dot{q}_1(t)) - L(q_2(t), \dot{q}_2(t)) + K(q_1(t), q_2(t), \dot{q}_1(t), \dot{q}_2(t))\right] \mathrm{d}t$$

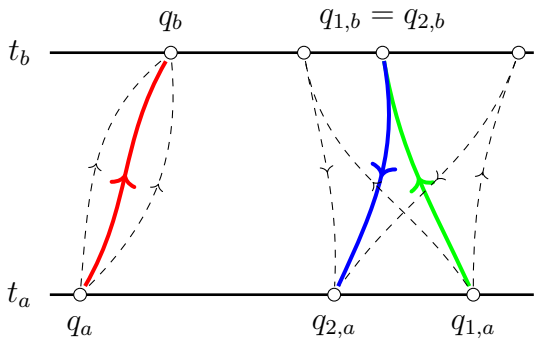


Figure 4.1: A mock-up comparison between the standard Hamilton's principle and Galley's modification. The arrows mark the direction in which the trajectory is traversed.

In particular, for the system we were considering we would have

$$\begin{aligned}\mathcal{J}_K[(q_1(t), q_2(t))] = \int_{t_a}^{t_b} \big[&L_{(\omega,m)}(q_1(t), \dot{q}_1(t)) - L_{(\omega,m)}(q_2(t), \dot{q}_2(t)) \\ &+ L_\lambda(q_1(t), \tilde{Q}_0(t)) - L_\lambda(q_2(t), \tilde{Q}_0(t)) \\ &+ K(q_1(t), q_2(t), \dot{q}_1(t), \dot{q}_2(t))\big]\,\mathrm{d}t\end{aligned}$$

with

$$\int_{t_a}^{t_b} K(q_1(t), q_2(t), \dot{q}_1(t), \dot{q}_2(t))\mathrm{d}t = \frac{\lambda^2}{2M}\int_{t_a}^{t_b}\int_{t_a}^{t_b}(q_1(t) - q_2(t))\widetilde{G}(t,s)(q_1(s) + q_2(s))\mathrm{d}s\mathrm{d}t$$

so q_1 and q_2 both couple to the retarded Green function in full, not just its symmetric part. To recuperate the right results, one needs to set $q_1 = q_2$, which Galley calls the *physical limit*. If the function $K(q_1, q_2, v_1, v_2)$ satisfies that $K(q_1, q_2, v_1, v_2) = -K(q_2, q_1, v_2, v_1)$, then it is possible to guarantee (see proposition 4.3.4) that in the physical limit the equations of motion for q_1 and q_2 are the same, and can be reinterpreted as equations of motion for the original variable q.

In fact, these new functions allow us to add any arbitrary force we want. What we will do now in the following sections is proceed to study the geometry behind these ideas and its application to the problem of the order of forced variational integrators. These sections are part of a pair of papers, one of them published [MS18b], and another at an internal preprint stage [MS19]. The reader should be aware that we changed the sign convention in those papers with respect to Galley's.

4.3 Mechanics and geometry of Galley's duplication

We have conscientiously decided to maintain a more geometry-oriented approach in this section by starting from the Hamiltonian side. This formulation is based on a groupoidal construction (see section 2.1.3), so the unacquainted reader may feel overwhelmed. Perhaps, a more sensible starting point for those will be section 4.3.3, where we discuss the Lagrangian side. There, groupoids are mentioned too but the bulk of the section can be understood without them.

4.3.1 Symplectic groupoids

Definition 4.3.1. A **symplectic groupoid** is a Lie groupoid $G \rightrightarrows Q$ (see section 2.1.3), such that

1. (G, ω_G) is a symplectic manifold,
2. the graph of $\mu : G_2 \to G$ is a Lagrangian submanifold of $(G, -\omega_G) \times (G, -\omega_G) \times (G, \omega_G)$.

If $G \rightrightarrows Q$ is a symplectic groupoid with symplectic form ω_G on G then one may prove that [see MW88]

1. $\dim G = 2 \dim Q$,
2. $\epsilon(Q)$ is a Lagrangian submanifold of (G, ω_G),
3. ι is an antisymplectomorphism of (G, ω_G),
4. $(\ker T_g\alpha)^\perp = \ker T_g\beta$, for $g \in G$, where

$$(\ker T_g\alpha)^\perp = \{v \in T_gG \,|\, \omega_G(v, u) = 0, \forall u \in \ker T_g\alpha\} \,,$$

that is, the symplectic orthogonal of $\ker T_g\alpha$.

Moreover, there exists a unique Poisson structure on Q such that $\alpha : G \to Q$ (respectively, $\beta : G \to Q$) is a Poisson (respectively, anti-Poisson) morphism.

Example 4.3.1. Let $G \rightrightarrows Q$ be a Lie groupoid, and let $A^*G \to Q$ be the dual vector bundle of the associated Lie algebroid AG. Then, the *cotangent groupoid* $T^*G \rightrightarrows A^*G$ is a symplectic groupoid with the canonical symplectic form ω_G. Given $\mu \in T^*_gG$, the source and target mappings are defined

$$\langle \tilde{\alpha}(\mu), X(\alpha(g))\rangle = \left\langle \mu, \overrightarrow{X}(g)\right\rangle, \quad \left\langle \tilde{\beta}(\mu), X(\beta(g))\right\rangle = \left\langle \mu, \overleftarrow{X}(g)\right\rangle$$

for all $X \in \Gamma(AG)$. [see CDW87; Mar05; MMS15, for more details and the definition of the remaining structural maps of this Lie groupoid.]

Proposition 4.3.1. *Let $G \rightrightarrows Q$ be a Lie groupoid and $Z \in \mathfrak{X}(G)$ a vector field invariant by the inversion, that is,*

$$T_g\iota(Z(g)) = Z(g^{-1}), \quad \forall g \in G \,.$$

Then, for all $q \in Q$,

$$Z(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q) \,.$$

Proof. For all $v_q \in A_qG$, consider an α-vertical curve $g : I \to G$ such that $v = \frac{\mathrm{d}g}{\mathrm{d}t}(0)$. Then

$$T_{(\epsilon(q),\epsilon(q))}\mu(0_q, v_q) = \frac{\mathrm{d}}{\mathrm{d}t}\mu(\epsilon(q), g(t))\bigg|_{t=0} = \frac{\mathrm{d}g}{\mathrm{d}t}(0) = v \,.$$

Also, for the β-vertical curve $g^{-1} : I \to G$ we have

$$T_{(\epsilon(q),\epsilon(q))}\mu(T_{\epsilon(q)}\iota(v), 0_q) = \frac{\mathrm{d}}{\mathrm{d}t}\mu(\iota(g(t)), \epsilon(q))\bigg|_{t=0} = T_{\epsilon(q)}\iota(v) \,.$$

Therefore,

$$T_{(\epsilon(q),\epsilon(q))}\mu(T_{\epsilon(q)}\iota(v), v) = v + T_{\epsilon(q)}\iota(v)\,.$$

Since $\mu(g^{-1}(t), g(t)) = \epsilon(\beta(g(t)))$, then

$$(T_{\epsilon(q)}\iota)(v) = -v + T_{\epsilon(q)}(\epsilon \circ \beta)(v)\,. \tag{4.2}$$

Using that

$$Z(\epsilon(q)) - T_{\epsilon(q)}(\epsilon \circ \alpha)(Z(\epsilon(q))) \in A_q G\,,$$

we can substitute it for v and then from expression (4.2):

$$T_{\epsilon(q)}\iota(Z(\epsilon(q))) + Z(\epsilon(q)) = T_{\epsilon(q)}(\epsilon \circ \alpha)(Z(\epsilon(q))) + T_{\epsilon(q)}(\epsilon \circ \beta)(Z(\epsilon(q)))\,,$$

meaning

$$T_{\epsilon(q)}\iota(Z(\epsilon(q))) + Z(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q)\,.$$

However, from the hypothesis about Z, we have that

$$T_{\epsilon(q)}\iota(Z(\epsilon(q))) = Z(\epsilon(q))\,.$$

Therefore

$$Z(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q)\,.$$

□

Proposition 4.3.2. *Let $G \rightrightarrows Q$ be a symplectic groupoid with symplectic form ω_G and $f : G \to \mathbb{R}$ a function such that $f \circ \iota = -f$. Then, the corresponding Hamiltonian vector field X_f*

$$\imath_{X_f}\omega_G = \mathrm{d}f\,,$$

verifies that $X_f(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q)$ for all $q \in Q$.

Proof. Since $\iota^*\omega = -\omega$ then for all $Y \in \mathfrak{X}(G)$

$$\langle \mathrm{d}f, Y\rangle = \omega_G(X_f, Y) = -\iota^*\omega_G(X_f, Y) = -\omega_G(\iota_* X_f, \iota_*(Y))\,,$$

but from the hypothesis we have that

$$\langle \mathrm{d}f, Y\rangle = -\langle \mathrm{d}(f \circ \iota), Y\rangle = -\langle \mathrm{d}f, \iota_*(Y)\rangle = -\omega_G(X_f, \iota_*(Y))\,.$$

Therefore, from proposition 4.3.1 we deduce that $X_f(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q)$. □

All the geometric constructions that follow are based on a particular case of Lie groupoid, the banal (or pair) groupoid $G \equiv Q \times Q \rightrightarrows Q$ with structural maps:

$$\begin{aligned} &\alpha_Q(q, q') = q, \quad \beta_Q(q, q') = q', \quad \epsilon_Q(q) = (q, q),\\ &\iota_Q(q, q') = (q', q), \quad \mu_Q((q, q'), (q', q'')) = (q, q'')\,. \end{aligned} \tag{4.3}$$

In this case, the Lie algebroid of $Q \times Q \rightrightarrows Q$ is isomorphic to the tangent bundle $\tau_Q : TQ \to Q$.

The associated symplectic groupoid is $T^*(Q\times Q) \rightrightarrows T^*Q$ with the canonical symplectic structure $\omega_{Q\times Q}$ of $T^*(Q \times Q)$ and with structural maps

$$\begin{aligned} &\alpha_{T^*Q}(\alpha_q, \beta_{q'}) = -\alpha_q, \quad \beta_{T^*Q}(\alpha_q, \beta_{q'}) = \beta_{q'}, \quad \epsilon_{T^*Q}(\alpha_q) = (\alpha_q, -\alpha_q),\\ &\iota_{T^*Q}(\alpha_q, \beta_{q'}) = (-\beta_{q'}, -\alpha_q), \quad \mu_{T^*Q}((\alpha_q, \beta_{q'}), (-\beta_{q'}, \gamma_{q''})) = (\alpha_q, \gamma_{q''})\,. \end{aligned}$$

Consider the map

$$\begin{array}{rccc} \Psi: & T^*(Q\times Q) & \to & T^*Q\times T^*Q \\ & (\alpha_q,\beta_{q'}) & \mapsto & (-\alpha_q,\beta_{q'})\,. \end{array}$$

Using this map we have an alternative structure of symplectic groupoid $T^*Q\times T^*Q \rightrightarrows T^*Q$ given by

$$\begin{array}{l} \mathrm{pr}_1(\alpha_q,\beta_{q'})=\alpha_q, \quad \mathrm{pr}_2(\alpha_q,\beta_{q'})=\beta_{q'}, \quad \epsilon(\alpha_q)=(\alpha_q,\alpha_q), \\ \iota(\alpha_q,\beta_{q'})=(\beta_{q'},\alpha_q), \quad \mu((\alpha_q,\beta_{q'}),(\beta_{q'},\gamma_{q''}))=(\alpha_q,\gamma_{q''})\,. \end{array}$$

We can see that Ψ is in fact a symplectomorphism, i.e. $\Psi^*(\omega_{Q\times Q})=\Omega_{Q\times Q}$, where

$$\Omega_{Q\times Q}=\mathrm{pr}_2^*\omega_Q-\mathrm{pr}_1^*\omega_Q$$

is a symplectic form. This form makes $(T^*Q\times T^*Q,\Omega_{Q\times Q})$ a symplectic groupoid.

4.3.2 Forced Hamiltonian dynamics as free dynamics by duplication

In this section we define a new unforced Hamiltonian system whose dynamical equations are related with the forced system (H,f^H).

Consider the symplectic groupoid $(T^*Q\times T^*Q,\Omega_{Q\times Q})$ defined in the previous section, and consider the Hamiltonian $\boldsymbol{H}:T^*Q\times T^*Q\to\mathbb{R}$ defined by

$$\boldsymbol{H}(\alpha_q,\beta_{q'})=\left(H\circ\mathrm{pr}_2-H\circ\mathrm{pr}_1\right)(\alpha_q,\beta_{q'})=H(\beta_{q'})-H(\alpha_q)\,.$$

Observe that this Hamiltonian satisfies that $\boldsymbol{H}\circ\iota=-\boldsymbol{H}$. Thus, we have the following

Lemma 4.3.1. *The Hamiltonian vector field $X_{\boldsymbol{H}}$ given by*

$$\imath_{X_{\boldsymbol{H}}}\Omega_{Q\times Q}=\mathrm{d}\boldsymbol{H}$$

satisfies:

i) $X_{\boldsymbol{H}}$ is tangent to $\epsilon(T^*Q)$;

ii) $X_{\boldsymbol{H}}|_{\epsilon(T^*Q)}=\epsilon_*(X_H)$.

Proof. See proposition 4.3.2. □

Observe that the proof of lemma 4.3.1 is quite straightforward when using coordinates. In fact, if we take adapted coordinates $(q^i,p_i;Q^i,P_i)$ on $T^*Q\times T^*Q$ then

$$\boldsymbol{H}(q^i,p_i;Q^i,P_i)=H(Q^i,P_i)-H(q^i,p_i)\ ,$$

and so

$$X_{\boldsymbol{H}}=\frac{\partial H}{\partial p_i}(q,p)\frac{\partial}{\partial q^i}-\frac{\partial H}{\partial q^i}(q,p)\frac{\partial}{\partial p_i}+\frac{\partial H}{\partial P_i}(Q,P)\frac{\partial}{\partial Q^i}-\frac{\partial H}{\partial Q^i}(Q,P)\frac{\partial}{\partial P_i}$$

which is obviously tangent to $\epsilon(T^*Q)$. This last space is locally given by the vanishing of the $2n$-constraints $Q^i-q^i=0$ and $P_i-p_i=0$ and moreover 4.3.1ii) follows immediately since $\epsilon(q^i,p_i)=(q^i,p_i;q^i,p_i)$.

Define $\mathbb{F}\boldsymbol{H}^{\times}(\alpha_q, \beta_{q'}) = (-\mathbb{F}H(\alpha_q), \mathbb{F}H(\beta_{q'}))$ with Hessian matrix:

$$\begin{pmatrix} -\dfrac{\partial^2 H}{\partial p_i \partial p_j}(q,p) & 0_{n\times n} \\ 0_{n\times n} & \dfrac{\partial^2 H}{\partial P_i \partial P_j}(Q,P) \end{pmatrix}.$$

The following lemma is trivial but it will be useful for us when going to the Lagrangian side.

Lemma 4.3.2. *The transformation $\mathbb{F}\boldsymbol{H}^{\times} : T^*Q \times T^*Q \to TQ \times TQ$ is a local diffeomorphism if and only if $\mathbb{F}H : T^*Q \to TQ$ is a local diffeomorphism.*

Given a Hamiltonian $\boldsymbol{H}$, we may want to add a *generalized potential* $\widetilde{\boldsymbol{K}} : T^*Q \times T^*Q \to \mathbb{R}$. This allows a richer behaviour of the original system in T^*Q. In light of the result of lemma 4.3.1, if this function has the property $\widetilde{\boldsymbol{K}} \circ \iota = -\widetilde{\boldsymbol{K}}$, then $\boldsymbol{H}_{\widetilde{\boldsymbol{K}}} = \boldsymbol{H} + \widetilde{\boldsymbol{K}}$ will still preserve that property and the trajectories of the resulting dynamics at the identities will remain bound to the identities.

The previous results are only a preparation for our real objective, which is to find a purely Hamiltonian representation of systems with forces using this duplication of variables.

In what follows, it will be interesting to introduce $\sigma : TQ \to Q \times Q$ defined by $\sigma(v_q) = (q, R_q(v_q))$, where R_q is a tangent retraction (see def.2.1.1). It is easy to show that σ is invertible in a neighborhood of $0_q \in T_qQ$ for any $q \in Q$. Denote this local inverse by $\tau : Q \times Q \to TQ$, which in coordinates will take the form

$$\tau(q^i, Q^i) = (q^i, \tau^i(q, Q)).$$

Lemma 4.3.3. *Consider a chart (U, φ) around a point $q \in Q$, then the map $\sigma : TU \to Q \times Q$ defined by $\sigma(v_q) = (q, R_q(v_q))$, where $q \in U$ satisfies that the map $T_{0_q}\sigma$ in coordinates $(TU, T\varphi)$ and $(U \times U, \varphi \times \varphi)$ is*

$$\begin{pmatrix} I & 0 \\ I & I \end{pmatrix}$$

and, in consequence, the map $T_{(q,q)}\tau$ is represented by the matrix

$$\begin{pmatrix} I & 0 \\ -I & I \end{pmatrix}.$$

Proof. We have that in the chosen coordinates $\sigma(q^i, v^i) = (F^i(q,v), G^i(q,v)) = (q, R_q(v))$. Therefore, in coordinates,

$$\frac{\partial F^i}{\partial q^j}(q,0) = \delta^i_j, \quad \frac{\partial F^i}{\partial v^j}(q,0) = 0,$$

where δ^i_j is the Kronecker delta, and observe that

$$\frac{\partial G^i}{\partial q^j}(q,0) = \delta^i_j$$

since $R_{q'}(0) = q'$ for $q' \in U$ and

$$\frac{\partial G^i}{\partial v^j}(q,0) = \delta^i_j$$

since $T_{0_q}R_q = \mathrm{id}_{T_qQ}$. □

Typically, we can induce this kind of mappings using an auxiliary Riemannian metric g on Q with associated geodesic spray Γ_g [see Car92]. The associated exponential for a small enough neighborhood $U \subset TQ$ of 0_q,

$$\begin{aligned} \exp^{\Gamma_g} : \ U \subset TQ &\to Q \times Q \\ v_q &\mapsto (q, \gamma_{v_q}(1)) \end{aligned}$$

where $t \to \gamma_{v_q}(t)$ is the unique geodesic such that $\gamma'_{v_q}(0) = v_q$. For instance, when $Q = \mathbb{R}^n$ and we take the Euclidean metric, we induce the map

$$\tau(q, q') = (q, q' - q) \quad \text{and} \quad \sigma(q, v) = (q, q + v) \, .$$

Given a forced Hamiltonian system (H, f^H), we can always construct the function $\widetilde{\boldsymbol{K}}_f : T^*Q \times T^*Q \to \mathbb{R}$ as:

$$\widetilde{\boldsymbol{K}}_f(\alpha_q, \beta_{q'}) = \frac{1}{2}\langle f^H(\beta_{q'}), \tau(q', q)\rangle - \frac{1}{2}\langle f^H(\alpha_q), \tau(q, q')\rangle \, .$$

Observe that this function satisfies the important property $\widetilde{\boldsymbol{K}}_f(\beta_{q'}, \alpha_q) = -\widetilde{\boldsymbol{K}}_f(\alpha_q, \beta_{q'})$, and thus is a generalized potential. Consider the Hamiltonian $\boldsymbol{H}_f : T^*Q \times T^*Q \to \mathbb{R}$ defined by

$$\boldsymbol{H}_f(\alpha_q, \beta_{q'}) = \boldsymbol{H}(\alpha_q, \beta_{q'}) + \widetilde{\boldsymbol{K}}_f(\alpha_q, \beta_{q'}) \, ,$$

which also satisfies $\boldsymbol{H}_f(\beta_{q'}, \alpha_q) = -\boldsymbol{H}_f(\alpha_q, \beta_{q'})$ by construction.

Note that we are not imposing that f^H be of any particular kind, so this approach is fairly general. Also note that this choice of generalized potential is not the only possible one. In fact, if a given f^H can be derived from a more fundamental theory, it may be entirely possible to derive a better suited $\widetilde{\boldsymbol{K}}$ from a Fokker effective action.

Theorem 4.3.4. *The Hamiltonian vector field $X_{\boldsymbol{H}_f}$ given by*

$$\imath_{X_{\boldsymbol{H}_f}} \Omega_{Q\times Q} = \mathrm{d}\boldsymbol{H}_f$$

satisfies:

i) $X_{\boldsymbol{H}_f}$ is tangent to $\epsilon(T^*Q)$;

ii) $X_{\boldsymbol{H}_f}\big|_{\epsilon(T^*Q)} = \epsilon_*(X_H + Y_f^v)$.

Proof. Part i) is again a direct consequence of proposition 4.3.2.

To deduce part ii) observe that

$$\begin{aligned} X_{\boldsymbol{H}_f} = &\left(\frac{\partial H}{\partial p_i}(q,p) + \frac{1}{2}\frac{\partial f_j^H}{\partial p_i}(q,p)\tau^j(q,Q)\right)\frac{\partial}{\partial q^i} \\ &- \left(\frac{\partial H}{\partial q^i}(q,p) + \frac{1}{2}\frac{\partial f_j^H}{\partial q^i}(q,p)\tau^j(q,Q)\right. \\ &\left. + \frac{1}{2}f_j^H(q,p)\frac{\partial \tau^j}{\partial q^i}(q,Q) - \frac{1}{2}f_j^H(Q,P)\frac{\partial \tau^j}{\partial q^i}(Q,q)\right)\frac{\partial}{\partial p_i} \\ &+ \left(\frac{\partial H}{\partial P_i}(Q,P) + \frac{1}{2}\frac{\partial f_j^H}{\partial P_i}(Q,P)\tau^j(Q,q)\right)\frac{\partial}{\partial Q^i} \\ &- \left(\frac{\partial H}{\partial Q^i}(Q,P) - \frac{1}{2}f_j^H(q,p)\frac{\partial \tau^j}{\partial Q^i}(q,Q)\right. \\ &\left. + \frac{1}{2}\frac{\partial f_j^H}{\partial Q^i}(Q,P)\tau^j(Q,q) + \frac{1}{2}f_j^H(Q,P)\frac{\partial \tau^j}{\partial Q^i}(Q,q)\right)\frac{\partial}{\partial P_i} \, . \end{aligned}$$

Now using lemma 4.3.3 we have that along the identities $\epsilon(T^*Q)$

$$X_{\boldsymbol{H}_f} = \frac{\partial H}{\partial p_i}(q,p)\frac{\partial}{\partial q^i} - \left(\frac{\partial H}{\partial q^i}(q,p) - f_j^H(q,p)\right)\frac{\partial}{\partial p_i} + \frac{\partial H}{\partial p_i}(q,p)\frac{\partial}{\partial Q^i} - \left(\frac{\partial H}{\partial q^i}(q,p) - f_j^H(q,p)\right)\frac{\partial}{\partial P_i}$$

and thus $X_{\boldsymbol{H}_f}\big|_{\epsilon(T^*Q)} = \epsilon_*(X_H + Y_f^v)$ as we wanted to prove. □

Define the mapping $\mathbb{F}\boldsymbol{H}_f^\times : T^*Q \times T^*Q \to TQ \times TQ$ given in adapted local coordinates as

$$\mathbb{F}\boldsymbol{H}_f^\times(q^i, p_i, Q^i, P_i) = \left(q^i, -\frac{\partial \boldsymbol{H}_f}{\partial p_i}, Q^i, \frac{\partial \boldsymbol{H}_f}{\partial P_i}\right).$$

Proposition 4.3.3. *If H is regular, then the transformation $\mathbb{F}\boldsymbol{H}_f^\times : T^*Q \times T^*Q \to TQ \times TQ$ is a local diffeomorphism in a neighborhood of $\epsilon(T^*Q)$.*

Proof. Locally, if we take coordinates (q^i, p_i, Q^i, P_i), then from the definition of K_f we observe that

$$\left(\frac{\partial^2 \widetilde{\boldsymbol{K}}_f}{\partial p_i \partial p_j}\right)\Big|_{\epsilon(T^*Q)} = \left(\frac{\partial^2 \widetilde{\boldsymbol{K}}_f}{\partial P_i \partial P_j}\right)\Big|_{\epsilon(T^*Q)} = \left(\frac{\partial^2 \widetilde{\boldsymbol{K}}_f}{\partial p_i \partial P_j}\right)\Big|_{\epsilon(T^*Q)} . = 0$$

Therefore, from the regularity of H it is trivial to derive the regularity of $\boldsymbol{H}_{\widetilde{\boldsymbol{K}}}$ on a tubular neighborhood of $\epsilon(T^*Q)$. □

4.3.3 Forced Lagrangian dynamics as free dynamics by duplication

Now we will define a new free Lagrangian system whose dynamical equations are related with the forced system (L, f).

Consider again the cartesian product $Q \times Q$. As we have seen, this is a Lie groupoid together with the structural maps defined in eqs.(4.3). The tangent bundle of a Lie groupoid $G \rightrightarrows M$ is itself a Lie groupoid over the tangent of the base manifold, i.e. $TG \rightrightarrows TM$, whose structural maps are the tangent of the originals. Therefore $T(Q\times Q) \equiv TQ \times TQ$ is a Lie groupoid over TQ. To keep the notation close to the former section, let us denote its canonical projections as $\widehat{\mathrm{pr}}_{1,2} : TQ \times TQ \to TQ$. If $(v_q, V_Q) \in TQ \times TQ$, then we have $\widehat{\mathrm{pr}}_1(v_q, V_Q) = v_q$ and $\widehat{\mathrm{pr}}_2(u_q, V_Q) = V_Q$. Consider also the maps

$$\begin{array}{rccc} \hat{\imath}: & TQ \times TQ & \to & TQ \times TQ \\ & (v_q, V_Q) & \mapsto & (V_Q, v_q) \end{array}$$

and

$$\begin{array}{rccc} \hat{\epsilon}: & TQ & \to & TQ \times TQ \\ & v_q & \mapsto & (v_q, v_q)\,. \end{array}$$

Multiplication can also be defined but will not be necessary for our purposes.

Clearly, $TQ \times TQ$ is equipped with a vertical endomorphism and a Liouville field, whose local presentation in adapted coordinates $(q^i, v^i; Q^i, V^i)$ are, respectively,

$$S = \mathrm{d}q^i \otimes \frac{\partial}{\partial v^i} + \mathrm{d}Q^i \otimes \frac{\partial}{\partial V^i},$$
$$\triangle = v^i \partial_{v^i} + V^i \partial_{V^i}.$$

Define a new Lagrangian $\boldsymbol{L} : TQ \times TQ \to \mathbb{R}$ as:

$$\boldsymbol{L}(v_q, V_Q) = (L \circ \widehat{\mathrm{pr}}_2 - L \circ \widehat{\mathrm{pr}}_1)(v_q, V_Q) = L(V_Q) - L(v_q)\,.$$

Much like $\boldsymbol{H}$, this new Lagrangian satisfies that $\boldsymbol{L} \circ \hat{\imath} = -\boldsymbol{L}$.

As with the Hamiltonian formulation, we may also include potentials in our description. Again, let $\boldsymbol{K} : TQ \times TQ \to \mathbb{R}$ be a function such that $\boldsymbol{K} \circ \hat{\imath} = -\boldsymbol{K}$, then $\boldsymbol{K}$ is a generalized potential and $\boldsymbol{L}_{\boldsymbol{K}} = \boldsymbol{L} - \boldsymbol{K}$ satisfies $\boldsymbol{L}_{\boldsymbol{K}} \circ \hat{\imath} = -\boldsymbol{L}_{\boldsymbol{K}}$.

The following general proposition states that in the particular case of Lagrangians satisfying this property, the identity set $\hat{\epsilon}(TQ)$ is an invariant set for the flow of its Euler-Lagrange equations.

Proposition 4.3.4. *Let $L : TQ \to \mathbb{R}$ be a regular Lagrangian and $\varphi : Q \to Q$ a diffeomorphism verifying that $L \circ \varphi_* = \pm L$. Denote by $M_\varphi = \{v_q \in Q \,|\, \varphi_*(v_q) = v_q\}$. Then M_φ is an invariant set for any solution of the Euler-Lagrange equations.*

Proof. Consider the action

$$\mathcal{J}[c] = \int_{t_a}^{t_b} L(c(t), \dot{c}(t))\,\mathrm{d}t\,,$$

with $c \in C^2(q_a, q_b, [t_a, t_b])$. As usual assume a family $c_\epsilon \in C^2(q_a, q_b, [t_a, t_b])$ such that

$$X(t) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} c_\epsilon(t)\bigg|_{\epsilon=0} \in T_c C^2(q_a, q_b, [t_a, t_b])\,.$$

We then have

$$\begin{aligned}\mathrm{d}\mathcal{J}[c](X) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{J}[c_\epsilon]\bigg|_{\epsilon=0} \\ &= \int_{t_a}^{t_b} \frac{\mathrm{d}}{\mathrm{d}\epsilon} L(c_\epsilon(t), \dot{c}_\epsilon(t))\,\bigg|_{\epsilon=0} \mathrm{d}t\,.\end{aligned}$$

Using that $L \circ \varphi = \pm L$

$$\begin{aligned}\mathrm{d}\mathcal{J}[c](X) &= \pm \int_{t_a}^{t_b} \frac{\mathrm{d}}{\mathrm{d}\epsilon} L\left(\varphi(c_\epsilon(t)), \frac{\mathrm{d}}{\mathrm{d}t}(\varphi(c_\epsilon(t)))\right)\bigg|_{\epsilon=0} \mathrm{d}t \\ &= \pm \frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} (\mathcal{J}[\varphi \circ c_\epsilon]) \\ &= \pm \mathrm{d}\mathcal{J}[\varphi \circ c](\varphi_* \circ X)\,.\end{aligned}$$

Observe that $\varphi_* \circ X \in T_{\varphi \circ c} C^2(\varphi(q_a), \varphi(q_b), [t_a, t_b])$. Since φ is a diffeomorphism then c is a critical point of $\mathcal{J}$ iff $\varphi \circ c$ is a critical point of $\mathcal{J}$.

Now, if $c : [t_a, t_b] \to Q$ is a solution of the Euler-Lagrange equations ($\mathrm{d}\mathcal{J}[c] = 0$) with $\dot{c}(t_a) \in M_\varphi$, then $\varphi \circ c$ is also a solution of the Euler-Lagrange equations. Observe that

$$\frac{\mathrm{d}(\varphi \circ c)}{\mathrm{d}t}(t_a) = \varphi_*(\dot{c}(t_a)) = \dot{c}(t_a)\,.$$

Consequently, $\varphi \circ c$ and c are solutions of the Euler-Lagrange equations with the same initial conditions. Since L is regular, it implies that $c = \varphi \circ c$ and $\dot{c}(t) \in M_\varphi$, for all t. □

With this result we can now state Hamilton's principle with initial values proposed by Galley in a more rigorous form.

Consider curves $\boldsymbol{c} : [t_a, t_b] \subseteq \mathbb{R} \to Q \times Q$ of class C^2 departing from a point $\boldsymbol{c}(t_a) = \boldsymbol{q}_a = (q_a, Q_a)$ with velocity $\boldsymbol{v}_a = (v_a, V_a) \in T_{\boldsymbol{c}(t_a)}(Q \times Q)$ and such that $\hat{\boldsymbol{c}}(t_b) \in \hat{\epsilon}(TQ)$, where $\hat{\boldsymbol{c}}$ is the tangent lift of $\boldsymbol{c}$ (see 2.1.2). Let us denote the collection of all these curves as

$$\boldsymbol{C}^2((\boldsymbol{q}_a, \boldsymbol{v}_a), [t_a, t_b]) = \left\{ \boldsymbol{c} : [t_a, t_b] \to Q \,|\, \boldsymbol{c} \in C^2([t_a, t_b]), \hat{\boldsymbol{c}}(t_a) = (\boldsymbol{q}_a, \boldsymbol{v}_a), \hat{\boldsymbol{c}}(t_b) \in \hat{\epsilon}(TQ) \right\},$$

and its tangent space as

$$T_{\boldsymbol{c}}\boldsymbol{C}^2((\boldsymbol{q}_a, \boldsymbol{v}_a), [t_a, t_b]) = \\ \left\{ \boldsymbol{X} : [t_a, t_b] \to T(Q \times Q) \,|\, \boldsymbol{X} \in C^1([t_a, t_b]), \tau_{Q\times Q} \circ \boldsymbol{X} = \boldsymbol{c}, \boldsymbol{X}(t_a) = 0, \boldsymbol{X}(t_b) \in \hat{\epsilon}(TQ) \right\}.$$

Let us also define an analogous space for curves $c : [t_a, t_b] \subseteq \mathbb{R} \to Q$, as

$$C^2((q_a, v_a), [t_a, t_b]) = \left\{ c : [t_a, t_b] \to Q \,|\, c \in C^2([t_a, t_b]), \hat{c}(t_a) = (q_a, v_a) \right\}.$$

Clearly if $\boldsymbol{c} \in \boldsymbol{C}^2((\boldsymbol{q}_a, \boldsymbol{v}_a), [t_a, t_b])$, then $\alpha_Q(\boldsymbol{c}) = c_\alpha \in C^2((q_a, v_a), [t_a, t_b])$ and $\beta_Q(\boldsymbol{c}) = c_\beta \in C^2((Q_a, V_a)[t_a, t_b])$.

Given a Lagrangian $L : TQ \to \mathbb{R}$ and a generalized potential $\boldsymbol{K} : T(Q \times Q) \equiv TQ \times TQ \to \mathbb{R}$ such that $\boldsymbol{L}_{\boldsymbol{K}} \circ \hat{\imath} = -\boldsymbol{L}_{\boldsymbol{K}}$, we define its *action functional* as

$$\begin{array}{rccl} \mathcal{J} : & \boldsymbol{C}^2((\boldsymbol{q}_a, \boldsymbol{v}_a), [t_a, t_b]) & \to & \mathbb{R} \\ & c & \mapsto & \int_{t_a}^{t_b} \boldsymbol{L}_{\boldsymbol{K}}(\hat{\boldsymbol{c}}(t)) \mathrm{d}t \,. \end{array}$$

By proposition 4.3.4, if $\boldsymbol{c}$ is a critical point of $\mathcal{J}[\boldsymbol{c}]$ such that $\hat{\boldsymbol{c}}(t_a) \in \hat{\epsilon}(TQ)$, then $\boldsymbol{c}(t) \in \epsilon_Q(Q)$ for all $t \in [t_a, t_b]$. Therefore, $\alpha_Q(\boldsymbol{c}) = \beta_Q(\boldsymbol{c}) = c$.

Definition 4.3.2. (Hamilton's principle with initial values). A curve $c \in C^2((q_a, v_a), [t_a, t_b])$ is the *physical trajectory* of a forced Lagrangian system defined by $L : TQ \to \mathbb{R}$ and a force $f : TQ \to T^*Q$ defined by

$$f = \mathrm{pr}_2 \left(\left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial \boldsymbol{K}}{\partial \dot{Q}} \right) - \frac{\partial \boldsymbol{K}}{\partial Q} \right) \circ \hat{\epsilon} \right) = \mathrm{pr}_1 \left(\left(-\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial \boldsymbol{K}}{\partial \dot{q}} \right) + \frac{\partial \boldsymbol{K}}{\partial q} \right) \circ \hat{\epsilon} \right)$$

if and only if $\epsilon_Q(c)$ is a critical point of the functional $\mathcal{J}$, i.e. $\mathrm{d}\mathcal{J}[\epsilon_Q(c)](\boldsymbol{X}) = 0$, for all $\boldsymbol{X} \in T_{\epsilon_Q(c)}\boldsymbol{C}^2((q_a, v_a), [t_a, t_b])$.

It is not difficult to show that a critical point of $\mathcal{J}$ is a curve $\boldsymbol{c}$ with local coordinates $\boldsymbol{c}(t) = (q^i(t), Q^i(t), \dot{q}^i(t), \dot{Q}^i(t))$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial \boldsymbol{L}}{\partial \dot{q}^i} \right) - \frac{\partial \boldsymbol{L}}{\partial q^i} = 0 \,, \quad \text{for } i = 1, ..., n \\ \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial \boldsymbol{L}}{\partial \dot{Q}^i} \right) - \frac{\partial \boldsymbol{L}}{\partial Q^i} = 0 \,, \end{aligned}$$

which in terms of L and $\boldsymbol{K}$, is

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = -\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial \boldsymbol{K}}{\partial \dot{q}^i} \right) + \frac{\partial \boldsymbol{K}}{\partial q^i} \,, \\ \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \dot{Q}^i} \right) - \frac{\partial L}{\partial Q^i} = \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial \boldsymbol{K}}{\partial \dot{Q}^i} \right) - \frac{\partial \boldsymbol{K}}{\partial Q^i} \,. \end{aligned}$$

When $\boldsymbol{c} \in \epsilon(Q)$, then c satisfies Hamilton's principle with initial values, and the equations of motion are precisely

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} &= \left(-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{K}}{\partial \dot{q}^i}\right) + \frac{\partial \boldsymbol{K}}{\partial q^i}\right) \circ \hat{\epsilon} \\ &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{K}}{\partial \dot{Q}^i}\right) - \frac{\partial \boldsymbol{K}}{\partial Q^i}\right) \circ \hat{\epsilon}\,.\end{aligned}$$

The Hamilton's principle with initial values is clearly equivalent to the standard Hamilton's principle once the variables have been duplicated, so we may continue using the latter.

Fibre derivatives and Poincaré-Cartan forms

From a generalized Lagrangian $\boldsymbol{L}$ we can define corresponding Poincaré-Cartan forms on $TQ \times TQ$, $\theta_{\boldsymbol{L}} = S^*(\mathrm{d}\boldsymbol{L})$ and $\omega_{\boldsymbol{L}} = -\mathrm{d}\theta_{\boldsymbol{L}}$, as in section 3.1.1. We can also define a new fibre derivative $\mathbb{F}\boldsymbol{L}^\times(v_q, V_Q) = (-\mathbb{F}L(v_q), \mathbb{F}L(V_Q))$. This leads us to state an analogue of lemma 4.3.2:

Lemma 4.3.5. *The transformation $\mathbb{F}\boldsymbol{L}^\times : TQ \times TQ \to T^*Q \times T^*Q$ is a local diffeomorphism if and only if $\mathbb{F}L : TQ \to T^*Q$ is a local diffeomorphism.*

It is easy to check that with this definition of fibre derivative the following diagram commutes:

$$\begin{array}{ccc} TQ \times TQ & \xrightarrow{\mathbb{F}\boldsymbol{L}^\times} & T^*Q \times T^*Q \\ {\scriptstyle\hat{\epsilon}}\uparrow & & \uparrow{\scriptstyle\epsilon} \\ TQ & \xrightarrow{\mathbb{F}L} & T^*Q \end{array}$$

This allows us to state the following

Proposition 4.3.5. *The regular Lagrangian $\boldsymbol{L}$ induces a symplectic structure on the Lie groupoid $TQ \times TQ \rightrightarrows TQ$, $\left(\mathbb{F}\boldsymbol{L}^\times\right)^* \Omega_{Q\times Q} = \omega_{\boldsymbol{L}}$, which makes $(TQ \times TQ, \omega_{\boldsymbol{L}})$ a symplectic groupoid.*

We can also define the energy of the system as in the usual case, with $E_{\boldsymbol{L}} = \triangle(\boldsymbol{L}) - \boldsymbol{L}$, but in order to relate this with the Hamiltonian formulation, it will be useful to rewrite it as:

$$E_{\boldsymbol{L}}(v_q, V_Q) = \left\langle \mathbb{F}\boldsymbol{L}^\times(v_q, V_Q), (v_q, V_Q) \right\rangle_\times - \boldsymbol{L}(v_q, V_Q)$$

where $\langle \cdot, \cdot \rangle_\times : (T^*Q \times T^*Q) \times (TQ \times TQ) \to \mathbb{R}$ is the inner product defined as:

$$\langle \alpha, v \rangle_\times = \langle \mathrm{pr}_2(\alpha), \widehat{\mathrm{pr}}_2(v) \rangle - \langle \mathrm{pr}_1(\alpha), \widehat{\mathrm{pr}}_1(v) \rangle\,.$$

The following results will help us prove the analogue of lemma 4.3.1.

Proposition 4.3.6. *Let $\boldsymbol{L} : TQ \times TQ \to \mathbb{R}$ be such that $\boldsymbol{L} \circ \hat{\imath} = -\boldsymbol{L}$, then the following diagram commutes:*

$$\begin{array}{ccc} TQ \times TQ & \xrightarrow{\mathbb{F}\boldsymbol{L}^\times} & T^*Q \times T^*Q \\ \downarrow{\scriptstyle\hat{\imath}} & & \downarrow{\scriptstyle\iota} \\ TQ \times TQ & \xrightarrow{\mathbb{F}\boldsymbol{L}^\times} & T^*Q \times T^*Q \end{array}$$

Proof. We need to show that:

$$\mathbb{F}\boldsymbol{L}^{\times} \circ \hat{\imath} = \iota \circ \mathbb{F}\boldsymbol{L}^{\times}.$$

On the left-hand side we have

$$\begin{aligned}\left(\mathbb{F}\boldsymbol{L}^{\times} \circ \hat{\imath}\right)(q, v, Q, V) &= \mathbb{F}\boldsymbol{L}^{\times}(Q, V, q, v) \\ &= \left(Q, -\frac{\partial \boldsymbol{L}}{\partial V}(Q, V, q, v), q, \frac{\partial \boldsymbol{L}}{\partial v}(Q, V, q, v)\right),\end{aligned}$$

while on the right-hand side we have

$$\begin{aligned}\left(\iota \circ \mathbb{F}\boldsymbol{L}^{\times}\right)(q, v, Q, V) &= \iota\left(q, -\frac{\partial \boldsymbol{L}}{\partial v}(q, v, Q, V), Q, \frac{\partial \boldsymbol{L}}{\partial V}(q, v, Q, V)\right) \\ &= \left(Q, \frac{\partial \boldsymbol{L}}{\partial V}(q, v, Q, V), q, -\frac{\partial \boldsymbol{L}}{\partial v}(q, v, Q, V)\right)\end{aligned}$$

Now, using that $\boldsymbol{L} \circ \hat{\imath} = -\boldsymbol{L}$ we find:

$$\begin{aligned}\frac{\partial \boldsymbol{L}}{\partial V}(Q, V, q, v) &= -\frac{\partial \boldsymbol{L}}{\partial V}(q, v, Q, V), \\ \frac{\partial \boldsymbol{L}}{\partial v}(Q, V, q, v) &= -\frac{\partial \boldsymbol{L}}{\partial v}(q, v, Q, V).\end{aligned}$$

Applying this we immediately arrive at the desired result. □

Lemma 4.3.6. *The inner product* $\langle \cdot, \cdot \rangle_{\times}$ *satisfies that*

$$\langle \iota(\alpha), \hat{\imath}(v) \rangle_{\times} = -\langle \alpha, v \rangle_{\times}.$$

Proof. First note that $\mathrm{pr}_1 \circ \iota = \mathrm{pr}_2$ and $\widehat{\mathrm{pr}}_1 \circ \hat{\imath} = \widehat{\mathrm{pr}}_2$, and that the same holds under the exchange $1 \leftrightarrow 2$.

Clearly:

$$\begin{aligned}\langle \iota(\alpha), \hat{\imath}(v) \rangle_{\times} &= \langle (\mathrm{pr}_2 \circ \iota)(\alpha), (\widehat{\mathrm{pr}}_2 \circ \hat{\imath})(v) \rangle - \langle (\mathrm{pr}_1 \circ \iota)(\alpha), (\widehat{\mathrm{pr}}_1 \circ \hat{\imath})(v) \rangle \\ &= \langle \mathrm{pr}_1(\alpha), \widehat{\mathrm{pr}}_1(v) \rangle - \langle \mathrm{pr}_2(\alpha), \widehat{\mathrm{pr}}_2(v) \rangle \\ &= -\langle \alpha, v \rangle_{\times}\end{aligned}$$

□

Proposition 4.3.7. *Let* $\boldsymbol{L}$ *be a Lagrangian such that* $\boldsymbol{L} \circ \hat{\imath} = -\boldsymbol{L}$*, then also* $E_{\boldsymbol{L}} \circ \hat{\imath} = -E_{\boldsymbol{L}}$*.*

Proof. Applying the inversion to the definition of the energy given in terms of $\mathbb{F}\boldsymbol{L}^{\times}$ we have:

$$\begin{aligned}\left(E_{\boldsymbol{L}} \circ \hat{\imath}\right)(\cdot) &= \left\langle (\mathbb{F}\boldsymbol{L}^{\times} \circ \hat{\imath})(\cdot), \hat{\imath}(\cdot) \right\rangle_{\times} - (\boldsymbol{L} \circ \hat{\imath})(\cdot) \\ &= \left\langle (\iota \circ \mathbb{F}\boldsymbol{L}^{\times})(\cdot), \hat{\imath}(\cdot) \right\rangle_{\times} - (\boldsymbol{L} \circ \hat{\imath})(\cdot)\end{aligned}$$

Applying lemma 4.3.6 and the inversion property of $\boldsymbol{L}$ we get:

$$\begin{aligned}\left(E_{\boldsymbol{L}} \circ \hat{\imath}\right)(\cdot) &= -\left\langle \mathbb{F}\boldsymbol{L}^{\times}(\cdot), \cdot \right\rangle_{\times} + \boldsymbol{L}(\cdot) \\ &= -E_{\boldsymbol{L}}(\cdot)\end{aligned}$$

□

Corollary 4.3.6.1. *Let $\boldsymbol{L}$ be a regular Lagrangian satisfying the hypothesis of proposition 4.3.6, and define its associated Hamiltonian by the expression $\boldsymbol{H} \circ \mathbb{F}\boldsymbol{L}^{\times} = E_{\boldsymbol{L}}$. Then $\boldsymbol{H} \circ \iota = -\boldsymbol{H}$.*

Proof. Using proposition 4.3.6 we have that $\boldsymbol{H} \circ \iota \circ \mathbb{F}\boldsymbol{L}^{\times} = \boldsymbol{H} \circ \mathbb{F}\boldsymbol{L}^{\times} \circ \hat{\iota} = E_{\boldsymbol{L}} \circ \hat{\iota}$. Applying proposition 4.3.7 the result follows immediately. □

Finally we can state the following result:

Proposition 4.3.8. *Assume L is a regular Lagrangian, then the Hamiltonian vector field $X_{E_{\boldsymbol{L}}}$ associated to $\boldsymbol{L}$ given by*

$$\imath_{X_{E_{\boldsymbol{L}}}} \omega_{\boldsymbol{L}} = \mathrm{d}E_{\boldsymbol{L}}$$

satisfies:

i) $X_{E_{\boldsymbol{L}}}$ is tangent to $\hat{\epsilon}(TQ)$;

ii) $X_{E_{\boldsymbol{L}}}|_{\hat{\epsilon}(TQ)} = \hat{\epsilon}_*(X_L)$.

Proof. We know that $\left(\mathbb{F}\boldsymbol{L}^{\times}\right)^* \Omega_{Q\times Q} = \omega_{\boldsymbol{L}}$. Defining $H = E_L \circ (\mathbb{F}L)^{-1}$ we then get that $\boldsymbol{H} = E_{\boldsymbol{L}} \circ \left(\mathbb{F}\boldsymbol{L}^{\times}\right)^{-1}$. Thus the results of lemma 4.3.1 also apply to $X_{E_{\boldsymbol{L}}}$ and these results can be brought back to $TQ \times TQ$, proving our claim. Variationally this is a direct consequence of proposition 4.3.4. □

Given a forced Lagrangian system (L, f) we may define the generalized potential $\boldsymbol{K}_f : TQ \times TQ \to \mathbb{R}$ explicitly written as:

$$\boldsymbol{K}_f(v_q, V_Q) = \frac{1}{2}\langle f(V_Q), \tau(Q, q)\rangle - \frac{1}{2}\langle f(v_q), \tau(q, Q)\rangle.$$

Note that if $\boldsymbol{L}_f = \boldsymbol{L} - \boldsymbol{K}_f$ is regular, we may obtain a Hamiltonian from its energy as $\boldsymbol{H}'_f = E_{\boldsymbol{L}_f} \circ \left(\mathbb{F}\boldsymbol{L}_f^{\times}\right)^{-1}$ but in general it will not be the same Hamiltonian as we defined in the previous section, i.e.

$$\widetilde{\boldsymbol{H}}_f \neq H \circ \mathrm{pr}_2 - H \circ \mathrm{pr}_1 + \frac{1}{2}\langle f^H \circ \mathrm{pr}_2, \tau \circ \pi_{Q\times Q} \circ \iota\rangle - \frac{1}{2}\langle f^H \circ \mathrm{pr}_1, \tau \circ \pi_{Q\times Q}\rangle\,.$$

This will only be equal if f does not depend on velocities, which means $\mathbb{F}\boldsymbol{L}_f^{\times} = \mathbb{F}\boldsymbol{L}^{\times}$. This means we cannot directly invoke the result from theorem 4.3.4 to prove that the resulting Euler-Lagrange field coincides with the forced dynamics at the identities and instead we must work a bit more to get the same result. Still at the end of the section we will show that we can actually relate both dynamics obtained from $\boldsymbol{H}_f$ and $\widetilde{\boldsymbol{H}}_f$.

Let us begin with this regularity result:

Proposition 4.3.9. *If L is regular, then $\boldsymbol{L}_f$ is regular in a neighborhood of $\hat{\epsilon}(TQ)$.*

Proof. The proof is essentially the same as that of proposition 4.3.3. □

Given $\boldsymbol{L}_{\boldsymbol{K}} = \boldsymbol{L} - \boldsymbol{K}$, with $\boldsymbol{L} = L \circ \widehat{\mathrm{pr}}_2 - L \circ \widehat{\mathrm{pr}}_1$, let us reserve $X_{E_{\boldsymbol{L}}}$ for the *free* Euler-Lagrange field, i.e. the vector field that satisfies

$$\imath_{X_{E_{\boldsymbol{L}}}} \omega_{\boldsymbol{L}} = \mathrm{d}E_{\boldsymbol{L}},$$

and define the vector field $Y_{\boldsymbol{K}}$ as the one resulting from the decomposition $X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}} = X_{E_{\boldsymbol{L}}} - Y_{\boldsymbol{K}}$. Similarly, let us define $\theta_{\boldsymbol{K}}$ by $\theta_{\boldsymbol{L}_{\boldsymbol{K}}} = \theta_{\boldsymbol{L}} - \theta_{\boldsymbol{K}}$ and $E_{\boldsymbol{K}}$ by $E_{\boldsymbol{L}_{\boldsymbol{K}}} = E_{\boldsymbol{L}} - E_{\boldsymbol{K}}$. Clearly, if $\omega_{\boldsymbol{K}} = -\mathrm{d}\theta_{\boldsymbol{K}}$, then $\omega_{\boldsymbol{L}_{\boldsymbol{K}}} = \omega_{\boldsymbol{L}} - \omega_{\boldsymbol{K}}$, and it is not difficult to show that:

$$\begin{aligned} \imath_{Y_{\boldsymbol{K}}}\omega_{\boldsymbol{L}_{\boldsymbol{K}}} &= \mathrm{d}E_{\boldsymbol{K}} - \imath_{X_{E_{\boldsymbol{L}}}}\omega_{\boldsymbol{K}} \\ &= \mathcal{L}_{X_{E_{\boldsymbol{L}}}}\theta_{\boldsymbol{K}} - \mathrm{d}\boldsymbol{K} \ . \end{aligned}$$

We can now prove the following theorem:

Theorem 4.3.7. *Given $\boldsymbol{L}_{\boldsymbol{K}} = \boldsymbol{L} - \boldsymbol{K}$ regular in a neighborhood of $\epsilon(TQ)$, with $\boldsymbol{L} = L \circ \widehat{\mathrm{pr}}_2 - L \circ \widehat{\mathrm{pr}}_1$, whose Hamiltonian vector field $X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}} = X_{E_{\boldsymbol{L}}} - Y_{\boldsymbol{K}}$ satisfies:*

$$\imath_{X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}}}\omega_{\boldsymbol{L}_{\boldsymbol{K}}} = \mathrm{d}E_{\boldsymbol{L}_{\boldsymbol{K}}} \tag{4.4}$$

then:

i) $X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}}$ is tangent to $\hat{\epsilon}(TQ)$;

ii) $Y_{\boldsymbol{K}}$ is vertical and such that $\hat{\imath}_* Y_{\boldsymbol{K}} = Y_{\boldsymbol{K}}$.

Furthermore, if $\boldsymbol{K} = \boldsymbol{K}_f$ and $\boldsymbol{L}_f = \boldsymbol{L} - \boldsymbol{K}_f$, then we have that:

iii) $\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{K}_f}\Big|_{\hat{\epsilon}(TQ)} = 0$;

iv) $\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{L}}\Big|_{\hat{\epsilon}(TQ)} = \left(\widehat{\mathrm{pr}}_1^* f - \widehat{\mathrm{pr}}_2^* f\right)|_{\hat{\epsilon}(TQ)}$;

v) $X_{E_{\boldsymbol{L}_f}}\Big|_{\hat{\epsilon}(TQ)} = \hat{\epsilon}_*(X_{E_L} + Z_f^v)$.

Proof. i) Geometrically, given the regularity in a neighborhood of the identities, $\omega_{\boldsymbol{L}_{\boldsymbol{K}}}$ is non-degenerate there. As $E_{\boldsymbol{L}_{\boldsymbol{K}}} \circ \hat{\imath} = -E_{\boldsymbol{L}_{\boldsymbol{K}}}$, we are in a position to apply proposition 4.3.2, rendering this equivalent to theorem 4.3.4.i). Variationally, the proof is a consequence of 4.3.4.

ii) We know that $X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}}$ and $X_{E_{\boldsymbol{L}}}$ are second order vector fields, as they solve their respective Euler-Lagrange equations. Thus, $S(X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}}) = S(X_{E_{\boldsymbol{L}}}) = \triangle$. Then necessarily $S(Y_{\boldsymbol{K}}) = 0$, which means it is vertical. As by proposition 4.3.8 both fields satisfy the symmetry property with respect to $\hat{\imath}$, $Y_{\boldsymbol{K}}$ must necessarily satisfy it too.

iii) For a general $\boldsymbol{K}$, using Cartan's magic formula we get that $\imath_{Y_{\boldsymbol{K}}}\omega_{\boldsymbol{K}} = \mathrm{d}\left(\imath_{Y_{\boldsymbol{K}}}\theta_{\boldsymbol{K}}\right) - \mathcal{L}_{Y_{\boldsymbol{K}}}\theta_{\boldsymbol{K}}$, but as we have just shown in ii), $Y_{\boldsymbol{K}}$ is vertical, and so $\imath_{Y_{\boldsymbol{K}}}\theta_{\boldsymbol{K}}$ vanishes identically. Thus, $\imath_{Y_{\boldsymbol{K}}}\omega_{\boldsymbol{K}} = -\mathcal{L}_{Y_{\boldsymbol{K}}}\theta_{\boldsymbol{K}}$. Now, if $Y_{\boldsymbol{K}} = Y_v^i\partial_{v^i} + Y_V^i\partial_{V^i}$ and $\theta_{\boldsymbol{K}} = \theta_i^q \mathrm{d}q^i + \theta_i^Q \mathrm{d}Q^i$, then:

$$\mathcal{L}_{Y_{\boldsymbol{K}}}\theta_{\boldsymbol{K}} = \left(Y_v^j\partial_{v^j} + Y_V^j\partial_{V^j}\right)\theta_i^q \mathrm{d}q^i + \left(Y_v^j\partial_{v^j} + Y_V^j\partial_{V^j}\right)\theta_i^Q \mathrm{d}Q^i \ .$$

In the special case of $\boldsymbol{K}_f$ we have that $\partial_{V^j}\theta_i^q = \partial_{v^j}\theta_i^Q = 0$, which reduces the former expression to:

$$\mathcal{L}_{Y_{\boldsymbol{K}_f}}\theta_{\boldsymbol{K}_f} = Y_v^j\partial_{v^j}\theta_i^q \mathrm{d}q^i + Y_V^j\partial_{V^j}\theta_i^Q \mathrm{d}Q^i \ .$$

Furthermore, $\partial_{v^j}\theta_i^q = -\frac{1}{2}\left\langle \frac{\partial^2 f}{\partial v^j \partial v^i}, \tau(q,Q)\right\rangle$, and similarly with $\partial_{V^j}\theta_i^Q$. As $\tau \circ \hat{\epsilon} = 0$, all these terms vanish at the identities.

iv) We know that $\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{L}} = \mathcal{L}_{X_{E_{\boldsymbol{L}_f}}}\theta_{\boldsymbol{K}_f} - \mathrm{d}\boldsymbol{K}_f + \imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{K}_f}$. We have just proven in iii) that at the identities the last term on the right-hand side vanishes. Thus, we only need to worry about the first and second terms. Proceeding as before, we can expand the Lie derivative with $X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}} = v^i\partial_{q^i} + V^i\partial_{Q^i} + X_v^i\partial_{v^i} + X_V^i\partial_{V^i}$:

$$\begin{aligned}\mathcal{L}_{X_{E_{\boldsymbol{L}_{\boldsymbol{K}}}}}\theta_{\boldsymbol{K}} = &\left(v^j\partial_{q^j} + V^j\partial_{Q^j} + X_v^j\partial_{v^j} + X_V^j\partial_{V^j}\right)\theta_i^q\mathrm{d}q^i \\ &+ \left(v^j\partial_{q^j} + V^j\partial_{Q^j} + X_v^j\partial_{v^j} + X_V^j\partial_{V^j}\right)\theta_i^Q\mathrm{d}Q^i \\ &+ \theta_j^q\partial_{v^i}v^j\mathrm{d}v^i + \theta_j^Q\partial_{V^i}V^j\mathrm{d}V^i\end{aligned}$$

Again, for $\boldsymbol{K} = \boldsymbol{K}_f$ we have that $\partial_{V^j}\theta_i^q = \partial_{v^j}\theta_i^Q = 0$, so simplifying this expression we get:

$$\begin{aligned}\mathcal{L}_{X_{E_{\boldsymbol{L}_f}}}\theta_{\boldsymbol{K}_f} = &\left(v^j\partial_{q^j} + V^j\partial_{Q^j} + X_v^j\partial_{v^j}\right)\theta_i^q\mathrm{d}q^i \\ &+ \left(v^j\partial_{q^j} + V^j\partial_{Q^j} + X_V^j\partial_{V^j}\right)\theta_i^Q\mathrm{d}Q^i \\ &+ \theta_i^q\mathrm{d}v^i + \theta_i^Q\mathrm{d}V^i\,.\end{aligned}$$

Under the same argument as in iii), the terms with derivatives in the v and V variables vanish at the identities. We can also see that $v^j\partial_{q^j}\theta_i^q + V^j\partial_{Q^j}\theta_i^q$ and its θ^Q counterpart must also vanish at the identities because:

$$\partial_Q\tau(q,q) = -\partial_q\tau(q,q)$$

Thus, $\mathcal{L}_{X_{E_{\boldsymbol{L}_f}}}\theta_{\boldsymbol{K}_f}\Big|_{\hat{\epsilon}(TQ)} = \left(\frac{\partial\boldsymbol{K}_f}{\partial v^i}\mathrm{d}v^i + \frac{\partial\boldsymbol{K}_f}{\partial V^i}\mathrm{d}V^i\right)\Big|_{\hat{\epsilon}(TQ)} = 0$. These also coincide with the v and V components of $\mathrm{d}\boldsymbol{K}$, so we only need to check what happens with the q and Q components:

$$\begin{aligned}\mathrm{d}\boldsymbol{K}_f = &\frac{1}{2}\left(\left\langle f(Q,V), \frac{\partial\tau}{\partial q^i}(Q,q)\right\rangle - \left\langle\frac{\partial f}{\partial q^i}(q,v), \tau(q,Q)\right\rangle\right. \\ &\left. - \left\langle f(q,v), \frac{\partial\tau}{\partial q^i}(q,Q)\right\rangle\right)\mathrm{d}q^i \\ &+ \frac{1}{2}\left(\left\langle\frac{\partial f}{\partial Q^i}(Q,V), \tau(Q,q)\right\rangle + \left\langle f(Q,V), \frac{\partial\tau}{\partial Q^i}(Q,q)\right\rangle\right. \\ &\left. - \left\langle f(q,v), \frac{\partial\tau}{\partial Q^i}(q,Q)\right\rangle\right)\mathrm{d}Q^i + \ldots\end{aligned}$$

At the identities all terms with a bare τ vanish, and using the properties of its derivatives, the remaining terms add up together forming $f_i(q,v)\mathrm{d}q^i - f_i(q,v)\mathrm{d}Q^i$.

v) Let us develop the left-hand side of iv):

$$\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{L}} = -\frac{\partial^2 L}{\partial v^j\partial v^i}Y_v^j\mathrm{d}q^i + \frac{\partial^2 L}{\partial V^j\partial V^i}Y_V^j\mathrm{d}Q^i$$

Restricting to $\hat{\epsilon}(TQ)$ and using iv) we get that:

$$Y_{\boldsymbol{K}_f}\big|_{\hat{\epsilon}(TQ)} = -(g_L)^{ij}\left(f_j\partial_{v^j} + f_j\partial_{V^j}\right) = \hat{\epsilon}_*(-Z_f^v)$$

where $(g_L)^{ij}$ are the entries of the inverse of the Hessian matrix of L, as defined in eq.(3.2).

□

Finding the integral curves of $X_{E_L} + Z_f^v$ is equivalent to solving the forced Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = f_i(q, \dot{q}^i) \, .$$

Then from theorem 4.3.7 we have that this is also equivalent to solving the unforced Lagrangian system derived by duplication given by $\boldsymbol{L}_f : TQ \times TQ \to \mathbb{R}$ and restricting the dynamics to $\hat{\epsilon}(TQ)$; in other words, it is equivalent to solving this system's Euler-Lagrange equations

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{L}_f}{\partial \dot{q}^i}\right) - \frac{\partial \boldsymbol{L}_f}{\partial q^i} &= 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{L}_f}{\partial \dot{Q}^i}\right) - \frac{\partial \boldsymbol{L}_f}{\partial Q^i} &= 0\end{aligned}$$

when restricted to $\hat{\epsilon}(TQ)$.

After theorem 4.3.7, the following result does not add much more, but gives us a better picture of the difference between the Hamiltonian and Lagrangian side and why the dynamics at the identities coincide:

Theorem 4.3.8. *Let (L, f) and (H, f^H) be a regular forced Lagrangian system and its associated forced Hamiltonian system, and denote by $\widetilde{\boldsymbol{H}}_f = E_{\boldsymbol{L}_f} \circ \left(\mathbb{F}\boldsymbol{L}_f^{\times}\right)^{-1}$ and $\boldsymbol{H}_f$ the corresponding generalized Hamiltonians. Then their respective Hamiltonian vector fields $X_{\widetilde{\boldsymbol{H}}_f}$ and $X_{\boldsymbol{H}_f}$ satisfy that $X_{\widetilde{\boldsymbol{H}}_f}\Big|_{\epsilon(T^*Q)} = X_{\boldsymbol{H}_f}|_{\epsilon(T^*Q)}$.*

Proof. Working on the Lagrangian side we know that $\boldsymbol{H}_f \circ \mathbb{F}\boldsymbol{L}^{\times} = E_{\boldsymbol{L}} + \boldsymbol{K}_f$, where $\mathbb{F}\boldsymbol{L}^{\times}$ is the fibre derivative induced by the free Lagrangian. This means that we have the following two concurrent dynamics:

$$\begin{aligned}\imath_{X_{E_{\boldsymbol{L}_f}}}\omega_{\boldsymbol{L}_f} &= \mathrm{d}E_{\boldsymbol{L}_f} \\ \imath_{\widehat{X}_{\boldsymbol{L}_f}}\omega_{\boldsymbol{L}} &= \mathrm{d}\left(E_{\boldsymbol{L}} + \boldsymbol{K}_f\right) \, .\end{aligned}$$

The respective transformed versions of the vector fields $X_{E_{\boldsymbol{L}_f}}$ and $\widehat{X}_{\boldsymbol{L}_f}$ are $X_{\widetilde{\boldsymbol{H}}_f}$ and $X_{\boldsymbol{H}_f}$. Clearly both $X_{E_{\boldsymbol{L}_f}}$ and $\widehat{X}_{\boldsymbol{L}_f}$ can be decomposed into $X_{E_{\boldsymbol{L}}} - Y_{\boldsymbol{K}_f}$ and $X_{E_{\boldsymbol{L}}} - \widehat{Y}_{\boldsymbol{K}_f}$ respectively. We are left with:

$$\begin{aligned}\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{L}_f} &= \mathcal{L}_{X_{E_{\boldsymbol{L}}}}\theta_{\boldsymbol{K}_f} - \mathrm{d}\boldsymbol{K}_f \\ \imath_{\widehat{Y}_{\boldsymbol{K}_f}}\omega_{\boldsymbol{L}} &= -\mathrm{d}\boldsymbol{K}_f \, .\end{aligned}$$

As we saw in proposition 4.3.7.iii), $\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{K}_f}\Big|_{\hat{\epsilon}(TQ)} = 0$, so we are left with:

$$\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{L}} = \mathcal{L}_{X_{E_{\boldsymbol{L}}}}\theta_{\boldsymbol{K}_f} - \mathrm{d}\boldsymbol{K}_f$$

and we saw in 4.3.7.iv) $\mathcal{L}_{X_{E_{\boldsymbol{L}}}}\theta_{\boldsymbol{K}_f}\Big|_{\hat{\epsilon}(TQ)} = 0$, thus $Y_{\boldsymbol{K}_f}\big|_{\hat{\epsilon}(TQ)} = \widehat{Y}_{\boldsymbol{K}_f}\Big|_{\hat{\epsilon}(TQ)}$. As both $\mathbb{F}\boldsymbol{L}_f^{\times}$ and $\mathbb{F}\boldsymbol{L}^{\times}$ coincide at the identities, then so will $X_{\widetilde{\boldsymbol{H}}_f}$ and $X_{\boldsymbol{H}_f}$, proving our claim. □

The two terms that must vanish at the identities for both dynamics to coincide, $\imath_{Y_{\boldsymbol{K}_f}}\omega_{\boldsymbol{K}_f}$ and $\mathcal{L}_{X_{E_{\boldsymbol{L}}}}\theta_{\boldsymbol{K}_f}$, amount to the condition that $\mathcal{L}_{X_{E_{\boldsymbol{L}_f}}}\theta_{\boldsymbol{K}_f}$ vanishes at the identities. This is still true for any $\boldsymbol{K}$ such that $\widetilde{\boldsymbol{K}} \circ \mathbb{F}\boldsymbol{L}^{\times} = \boldsymbol{K}$.

4.4 Variational order for forced discrete Lagrangian systems

4.4.1 Discrete Lagrangian dynamics obtained by duplication

We have a regular system defined by $\boldsymbol{L_K} : TQ \times TQ \to \mathbb{R}$. Now we consider a discretization of this Lagrangian

$$\boldsymbol{L_K^d} : Q \times Q \times Q \times Q \to \mathbb{R}$$

such that $\boldsymbol{L_K^d} = -\boldsymbol{L_K^d} \circ \hat{\imath}_d$ where $\hat{\imath}_d : Q \times Q \times Q \times Q \to Q \times Q \times Q \times Q$ is the inversion defined by

$$\hat{\imath}_d(q_k, q_{k+1}, Q_k, Q_{k+1}) = (Q_k, Q_{k+1}, q_k, q_{k+1}) \,.$$

Additionally, define the identity map $\hat{\epsilon}_d : Q \times Q \to Q \times Q \times Q \times Q$ by

$$\hat{\epsilon}_d(q_k, q_{k+1}) = (q_k, q_{k+1}, q_k, q_{k+1}) \,.$$

As we are studying discrete variational systems with a discrete symmetry, the following proposition will be useful later on.

Proposition 4.4.1. *Let $L_d : Q \times Q \to \mathbb{R}$ be a regular discrete Lagrangian and $\varphi_d : Q \to Q$ a diffeomorphism verifying that $L_d \circ (\varphi_d \times \varphi_d) = \pm L_d$. Denote by $M_{\varphi_d} = \{(q, q') \in Q \,|\, \varphi_d(q) = q, \varphi_d(q') = q'\}$. Then F_{φ_d} is an invariant set for any solution of the discrete Euler-Lagrange equations.*

Proof. The proof is similar to that of proposition 4.3.4.

Consider the discrete action

$$\mathcal{J}_d[c_d] = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$$

where $c_d \in C_d\,(q_a, q_b, T_d)$, with $q_a = q_0$ and $q_b = q_N$.

The extremals are characterized as the solutions of the discrete Euler-Lagrange equations:

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \quad \text{for } k = 1, ..., N-1 \,.$$

Then, it is clear that if $\{q_k\}_{k=1}^N$ is a solution of the discrete Euler-Lagrange equations, then from the invariance of L_d we easily derive that $\{\varphi_d(q_k)\}_{k=0}^N$ is also a solution with boundary conditions $\varphi_d(q_0)$ and $\varphi_d(q_N)$.

Therefore, if L_d is regular we have defined its discrete flow or discrete Lagrangian map:

$$\begin{array}{rccc} F_{L_d} : & Q \times Q & \to & Q \times Q \\ & (q_{k-1}, q_k) & \mapsto & (q_k, q_{k+1}) \,. \end{array}$$

Observe that also $F_{L_d}(\varphi_d(q_{k-1}), \varphi_d(q_k)) = (\varphi_d(q_k), \varphi_d(q_{k+1}))$. Now starting from initial conditions $(q_0, q_1) \in M_{\varphi_d}$, that is, $\varphi_d(q_0) = q_1, \varphi_d(q_1) = q_1$ from the uniqueness of solutions of the discrete Euler-Lagrange equations we obtain that $(q_{k-1}, q_k) \in M_{\varphi_d}$, $k = 1, ..., N$ and, as a consequence, M_{φ_d} is an invariant set of the discrete Euler-Lagrange equations. □

Theorem 4.4.1. *The flow $F_{\boldsymbol{L_K^d}} : Q \times Q \times Q \times Q \to Q \times Q \times Q \times Q$ defined by a discrete Lagrangian $\boldsymbol{L_K^d} : Q \times Q \times Q \times Q \to \mathbb{R}$ verifying that $\boldsymbol{L_K^d} = -\boldsymbol{L_K^d} \circ \hat{\imath}_d$ restricts to $\hat{\epsilon}_d(Q \times Q)$, that is,*

$$F_{\boldsymbol{L_K^d}} \circ \hat{\epsilon}_d(Q \times Q) \in \hat{\epsilon}_d(Q \times Q) \,.$$

Proof. The proof is a consequence of proposition 4.4.1. □

Now, we are in a position to state our main result.

Theorem 4.4.2. *Let (L, f) be a forced Lagrangian system. Derive from it the extended regular Lagrangian $\boldsymbol{L}_f : TQ \times TQ \to \mathbb{R}$ and consider the exact discrete extended Lagrangian*

$$\boldsymbol{L}_f^e(q_0, Q_0, q_1, Q_1) = \int_0^h \boldsymbol{L}_f(q_{0,1}(t), \dot{q}_{0,1}(t), Q_{0,1}(t), \dot{Q}_{0,1}(t))\, dt$$

where $t \mapsto (q_{0,1}(t), \dot{q}_{0,1}(t), Q_{0,1}(t))$ is the unique solution of the Euler-Lagrange equations for $\boldsymbol{L}_f$ satisfying $q_{0,1}(0) = q_0, Q_{0,1}(0) = Q_0, q_{0,1}(h) = q_1, Q_{0,1}(h) = Q_1$ and satisfying additionally that $\boldsymbol{L}_f^d \circ \hat{\imath}_d = -\boldsymbol{L}_f^d$.

If $\boldsymbol{L}_f^d : TQ \times TQ \to \mathbb{R}$ is a discretization of order r of $\boldsymbol{L}_f^e$ (see def. 3.2.2), then the discrete Euler-Lagrange equations of $\boldsymbol{L}_f^d$ restricted to $\hat{\epsilon}_d(Q \times Q)$ give us a numerical integrator of order r for the flow of the forced Lagrangian system (L, f).

Example 4.4.1. As an example consider a Lagrangian $L : \mathbb{R}^{2n} \to \mathbb{R}$:

$$L(q, v) = \frac{1}{2} v^T M v - \frac{1}{2} q^T K q\,,$$

and a dissipation force $f(q^i, v^i) = (q^i, -D_{ij} v^j)$.

The forced Euler-Lagrange equations are:

$$M\ddot{q}(t) + D\dot{q}(t) + Kq(t) = 0\,.$$

We will derive the extended Lagrangian $\boldsymbol{L}_f : \mathbb{R}^{4n} \to \mathbb{R}$. For that, we consider the function:

$$\boldsymbol{K}_f(q, v, Q, V) = -\frac{1}{2} DV \cdot (q - Q) + \frac{1}{2} Dv \cdot (Q - q) = \left[\frac{D}{2}(V + v)\right]^T (Q - q)\,.$$

Then

$$\begin{aligned}\boldsymbol{L}_f(q, v, Q, V) &= L(Q, V) - L(q, v) - \boldsymbol{K}_f(q, v, Q, V) \\ &= \frac{1}{2} V^T M V - \frac{1}{2} Q^T K Q - \frac{1}{2} v^T M v + \frac{1}{2} q^T K q - \left[\frac{D}{2}(V + v)\right]^T (Q - q)\,.\end{aligned}$$

By construction $\boldsymbol{L}_f(q, v, Q, V) = -\boldsymbol{L}_f(Q, V, q, v)$.

Let us discretize by applying the *midpoint rule*:

$$q \approx \frac{q_0 + q_1}{2}, \quad \dot{q} \approx \frac{q_1 - q_0}{h}$$

which leads to:

$$\begin{aligned}\boldsymbol{L}_f^d = &\frac{h}{2}\left(\frac{Q_{k+1} - Q_k}{h}\right)^T M \left(\frac{Q_{k+1} - Q_k}{h}\right) - \frac{h}{2}\left(\frac{Q_k + Q_{k+1}}{2}\right)^T K \left(\frac{Q_k + Q_{k+1}}{2}\right) \\ &- \frac{h}{2}\left(\frac{q_{k+1} - q_k}{h}\right)^T M \left(\frac{q_{k+1} - q_k}{h}\right) + \frac{h}{2}\left(\frac{q_k + q_{k+1}}{2}\right)^T K \left(\frac{q_k + q_{k+1}}{2}\right) \\ &- \frac{h}{2}\left[D\left(\frac{Q_{k+1} - Q_k}{h} + \frac{q_{k+1} - q_k}{h}\right)\right]^T \left(\frac{Q_k + Q_{k+1}}{2} - \frac{q_k + q_{k+1}}{2}\right)\,.\end{aligned}$$

Observe that

$$\boldsymbol{L}_f^d(q_k, Q_k, q_{k+1}, Q_{k+1}) = -\boldsymbol{L}_f^d(Q_k, q_k, Q_{k+1}, q_{k+1})\,.$$

Therefore, from theorem 4.4.2 this leads to a second order method restricting the discrete Euler-Lagrange equations to $\hat{\epsilon}_d(Q \times Q)$. The resulting equations are not very surprising:

$$M\left(\frac{Q_{k+2} - 2Q_{k+1} + Q_k}{h^2}\right) + D\left(\frac{Q_{k+2} - Q_k}{2h}\right) + K\left(\frac{Q_{k+2} + 2Q_{k+1} + Q_k}{4}\right) = 0\,.$$

The following results provide a purely variational base for the exact discrete forcing offered by Marsden and West, and show that usual Runge-Kutta type discretization schemes provide the same results as in their article.

Proposition 4.4.2. *The exact discrete Lagrangian defined by $\boldsymbol{L}_f^e(u_q, v_{q'})$ at the identities is equivalent to two copies of the one defined in [MW01, eq.(3.2.7)].*

Proof. The corresponding parts for L need not be checked as they correspond trivially to those of eq.(3.2.7a) with the adequate change of notation. It remains to show that $\boldsymbol{K}_f$ generates the *exact discrete forces* f_d^{e+}, f_d^{e-}.

The contribution of some K to the exact discrete Lagrangian is:

$$\boldsymbol{K}_d^e(q_0, Q_0, q_1, Q_1) = \int_0^h \boldsymbol{K}(q(t), v(t), Q(t), V(t))\mathrm{d}t \tag{4.5}$$

where $t \mapsto (q(t), Q(t)) \in Q \times Q$ is the unique solution for $\boldsymbol{L}_{\boldsymbol{K}_f}$ with boundary conditions $q(0) = q_0, Q(0) = Q_0, q(h) = q_1, Q(h) = Q_1$.

In the case where $\boldsymbol{K} = \boldsymbol{K}_f$, differentiating $\boldsymbol{K}_d$ with respect to q_0 we get:

$$\begin{aligned} &D_1\boldsymbol{K}_{f,d}^e(q_0, Q_0, q_1, Q_1) \\ &= \int_0^h \left[D_1\boldsymbol{K}_f \cdot \frac{\partial q(t)}{\partial q_0} + D_2\boldsymbol{K}_f \cdot \frac{\partial v(t)}{\partial q_0} + D_3\boldsymbol{K}_f \cdot \frac{\partial Q(t)}{\partial q_0} + D_4\boldsymbol{K}_f \cdot \frac{\partial V(t)}{\partial q_0}\right]\mathrm{d}t \end{aligned} \tag{4.6}$$

where:

$$\begin{aligned} D_1\boldsymbol{K}_f &= \frac{1}{2}\left[\langle f(Q,V), D_2\tau(Q,q)\rangle - \langle D_1 f(q,v), \tau(q,Q)\rangle - \langle f(q,v), D_1\tau(q,Q)\rangle\right] \\ D_2\boldsymbol{K}_f &= -\frac{1}{2}\langle D_2 f(q,v), \tau(q,Q)\rangle \\ D_3\boldsymbol{K}_f &= \frac{1}{2}\left[\langle D_1 f(Q,V), \tau(Q,q)\rangle + \langle f(Q,V), D_1\tau(Q,q)\rangle - \langle f(q,v), D_2\tau(q,Q)\rangle\right] \\ D_4\boldsymbol{K}_f &= \frac{1}{2}\langle D_2 f(Q,V), \tau(Q,q)\rangle\,. \end{aligned}$$

Similar expressions are found after differentiation with respect to q_0', q_1 and q_1'. Now, when restricted to the identities, we find that:

$$\begin{aligned} \hat{\epsilon}^* D_1\boldsymbol{K}_f &= \left\langle f(q,v), \mathrm{id}_{T_qQ}\right\rangle \\ \hat{\epsilon}^* D_2\boldsymbol{K}_f &= 0 \\ \hat{\epsilon}^* D_3\boldsymbol{K}_f &= -\left\langle f(q,v), \mathrm{id}_{T_qQ}\right\rangle \\ \hat{\epsilon}^* D_4\boldsymbol{K}_f &= 0 \end{aligned}$$

where we used the fact that $\tau(q,q) = 0_q$ and $\hat{\epsilon}^* D_2\tau = -\hat{\epsilon}^* D_1\tau = -\mathrm{id}_{T_qQ}$. This leads to:

$$\hat{\epsilon}_d^* D_1 \boldsymbol{K}_{f,d}^e = -\hat{\epsilon}_d^* D_2 \boldsymbol{K}_{f,d}^e = \int_0^h f(q(t),u(t)) \cdot \frac{\partial q(t)}{\partial q_0} \mathrm{d}t = f_d^{e-} \tag{4.7}$$

$$\hat{\epsilon}_d^* D_3 \boldsymbol{K}_{f,d}^e = -\hat{\epsilon}_d^* D_4 \boldsymbol{K}_{f,d}^e = \int_0^h f(q(t),u(t)) \cdot \frac{\partial q(t)}{\partial q_1} \mathrm{d}t = f_d^{e+} \,. \tag{4.8}$$

Putting everything together we find two copies of the forced discrete equations with opposite sign, which is what we set out to prove. □

Proposition 4.4.3. *Let (b_i, c_i) be some quadrature coefficients and let γ be a Galerkin-type interpolation polynomial associated to the coefficients c_i. Let us also use for convenience the notation $\gamma(t,q_0,q_1) = (\chi(t,q_0,q_1), \psi(t,q_0,q_1))$, with $\chi(t,q_0,q_1) \in Q$ and $\psi(t,q_0,q_1)) \in T_{\chi(t,q_0,q_1)}Q$ for each $t = [0,1]$. If we approximate the conservative discrete Lagrangian L as*

$$L_d(q_0,q_1) = h \sum_{i=1}^s b_i L \circ \gamma(c_i,q_0,q_1) \,,$$

then the contribution of $\boldsymbol{K}_f$, as defined in proposition 4.4.2, to the discrete Lagrangian $\boldsymbol{L}_f^d$ at the identities becomes:

$$\begin{aligned}
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_f^d}{\partial q_0} &= -h \sum_{i=1}^s b_i \left\langle f \circ \gamma(c_i,q_0,q_1), \frac{\partial \chi(c_i,q_0,q_1)}{\partial q_0} \right\rangle \\
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_f^d}{\partial Q_0} &= h \sum_{i=1}^s b_i \left\langle f \circ \gamma(c_i,q_0,q_1), \frac{\partial \chi(c_i,q_0,q_1)}{\partial q_0} \right\rangle \\
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_f^d}{\partial q_1} &= -h \sum_{i=1}^s b_i \left\langle f \circ \gamma(c_i,q_0,q_1), \frac{\partial \chi(c_i,q_0,q_1)}{\partial q_1} \right\rangle \\
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_f^d}{\partial Q_1} &= h \sum_{i=1}^s b_i \left\langle f \circ \gamma(c_i,q_0,q_1), \frac{\partial \chi(c_i,q_0,q_1)}{\partial q_1} \right\rangle \,.
\end{aligned}$$

Proof. For the contribution of $\boldsymbol{K}_f$ to the discrete Lagrangian we have:

$$\boldsymbol{K}_f^d(q_0,Q_0,q_1,Q_1) = h \sum_{i=1}^s b_i \boldsymbol{K}(\gamma(c_i,q_0,q_1), \gamma(c_i,Q_0,Q_1)) \,.$$

Differentiating with respect to q_0, q_0', q_1 and q_1' we have:

$$\begin{aligned}
\frac{\partial \boldsymbol{K}_f^d}{\partial q_0} &= h \sum_{i=1}^s b_i \left[D_1 K \cdot \frac{\partial \chi(c_i,q_0,q_1)}{\partial q_0} + D_2 K \cdot \frac{\partial \psi(c_i,q_0,q_1)}{\partial q_0} \right] \\
\frac{\partial \boldsymbol{K}_f^d}{\partial Q_0} &= h \sum_{i=1}^s b_i \left[D_3 K \cdot \frac{\partial \chi(c_i,Q_0,Q_1)}{\partial Q_0} + D_4 K \cdot \frac{\partial \psi(c_i,Q_0,Q_1)}{\partial Q_0} \right] \\
\frac{\partial \boldsymbol{K}_f^d}{\partial q_1} &= h \sum_{i=1}^s b_i \left[D_1 K \cdot \frac{\partial \chi(c_i,q_0,q_1)}{\partial q_1} + D_2 K \cdot \frac{\partial \psi(c_i,q_0,q_1)}{\partial q_1} \right] \\
\frac{\partial \boldsymbol{K}_f^d}{\partial Q_1} &= h \sum_{i=1}^s b_i \left[D_3 K \cdot \frac{\partial \chi(c_i,Q_0,Q_1)}{\partial Q_1} + D_4 K \cdot \frac{\partial \psi(c_i,Q_0,Q_1)}{\partial Q_1} \right]
\end{aligned}$$

where D_iK are the same as those of proposition 4.4.2 with $q(t) = \chi(t, q_0, q_1)$, $v(t) = \psi(t, q_0, q_1)$, $Q(t) = \chi(t, Q_0, Q_1)$, $V(t) = \psi(t, Q_0, Q_1)$. Restriction to the identities proves our claim. □

Example 4.4.2. Let us choose our discretisation to be:

$$L_d^\alpha(q_0, q_1) = hL\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right)$$

as in [MW01, example 3.2.2]. This results in:

$$\begin{aligned}
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_{f,d}^\alpha}{\partial q_0} &= h(1-\alpha) f\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right) \\
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_{f,d}^\alpha}{\partial Q_0} &= -h(1-\alpha) f\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right) \\
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_{f,d}^\alpha}{\partial q_1} &= h\alpha f\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right) \\
\hat{\epsilon}_d^* \frac{\partial \boldsymbol{K}_{f,d}^\alpha}{\partial Q_1} &= -h\alpha f\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right)
\end{aligned}$$

which coincides with their result.

In section 3.2.5 we also saw how to construct VPRK methods, which will play a very important role in chapter 5. We can easily do the same here, but we need to change our notation slightly, given that q and Q have different meanings there.

Consider then coordinates $(q_1, v_1, q_2, v_2) \in TQ \times TQ$ and denote $\boldsymbol{q} = (q_1, q_2)$, $\boldsymbol{v} = (v_1, v_2)$. Choose an s-stage RK scheme with $T_d = \{t_k\}_{k=0}^N$ such that $t_{k+1} - t_k = h$ and consider the space of s-stage variationally partitioned RK (s-stage VPRK) sequences:

$$\begin{aligned}
&\boldsymbol{C}_d^s(\boldsymbol{q}_a, \boldsymbol{q}_b) \\
&= \left\{ \left(\boldsymbol{q}, \tilde{\boldsymbol{p}}, \left\{ \boldsymbol{Q}^i, \boldsymbol{V}^i, \tilde{\boldsymbol{P}}^i \right\}_{i=1}^s \right) : T_d \to T^*Q \times T^*Q \times (\mathbb{T}Q \times \mathbb{T}Q)^s \mid \right. \\
&\left. \boldsymbol{q}(t_a = t_0) = \boldsymbol{q}_a, \boldsymbol{q}(t_b = t_N) = \boldsymbol{q}_b \right\}.
\end{aligned}$$

If $\boldsymbol{c}_d$, then let us denote by $\widehat{\mathrm{pr}}_i \boldsymbol{c}_d = c_{d,i}$, with $i = 1, 2$ a pair of curves in $C_d^s(q_{i,a}, q_{i,b})$ with components $\left(q_i, \tilde{p}_i, \left\{ Q_i^j, V_i^j, \tilde{P}_i^j \right\}_{j=1}^s \right)$. Let us also denote by $\hat{\imath} \boldsymbol{c}_d$ the unique discrete curve such that $\widehat{\mathrm{pr}}_1 \hat{\imath} \boldsymbol{c}_d = \widehat{\mathrm{pr}}_2 \boldsymbol{c}_d$ and $\widehat{\mathrm{pr}}_2 \hat{\imath} \boldsymbol{c}_d = \widehat{\mathrm{pr}}_1 \boldsymbol{c}_d$.

Then we can define the following discrete Hamilton-Pontryagin functional / extended cost functional $(\mathcal{J}_{\mathcal{HP}})_d : \boldsymbol{C}_d^s(\boldsymbol{q}_a, \boldsymbol{q}_b) \to \mathbb{R}$, by:

$$\begin{aligned}
(\mathcal{J}_{\mathcal{HP}})_d [\boldsymbol{c}_d] = \sum_{k=0}^{N-1} \sum_{i=1}^{s} hb_i \Bigg[& \boldsymbol{L}\left(Q_{1,k}^i, V_{1,k}^i, Q_{2,k}^i, V_{2,k}^i\right) + \left\langle \tilde{P}_{2,k}^i, \frac{Q_{2,k}^i - q_{2,k}}{h} - \sum_{j=1}^s a_{ij} V_{2,k}^j \right\rangle \\
& - \left\langle \tilde{P}_{1,k}^i, \frac{Q_{1,k}^i - q_{1,k}}{h} - \sum_{j=1}^s a_{ij} V_{1,k}^j \right\rangle + \left\langle \tilde{p}_{2,k+1}, \frac{q_{2,k+1} - q_{2,k}}{h} - \sum_{j=1}^s b_j V_{2,k}^j \right\rangle \\
& - \left\langle \tilde{p}_{1,k+1}, \frac{q_{1,k+1} - q_{1,k}}{h} - \sum_{j=1}^s b_j V_{1,k}^j \right\rangle \Bigg].
\end{aligned}$$

Theorem 4.4.3. *Let (L, f) be a regular Lagrangian forced system with $L : TQ \to \mathbb{R}$, C^ℓ with $\ell \geq 2$, and forcing $f : TQ \to T^*Q$. Let $\boldsymbol{L}_f : TQ \times TQ \to \mathbb{R}$ denote its associated generalized Lagrangian function satisfying that $\boldsymbol{L}_f \circ \hat{\imath} = -\boldsymbol{L}_f$. Let also $\boldsymbol{c}_d \in \boldsymbol{C}_d^s(\boldsymbol{q}_0, \boldsymbol{q}_N)$ be an s-stage VPRK sequence satisfying that $\boldsymbol{q}_0, \boldsymbol{q}_N \in \epsilon(TQ)$. Then $\boldsymbol{c}_d$ is a critical point of the discrete Hamilton-Pontryagin functional, $(\mathcal{J}_{\mathcal{HP}})_d$, if and only if $\widehat{\mathrm{pr}}_1 \boldsymbol{c}_d = \widehat{\mathrm{pr}}_2 \boldsymbol{c}_d = c_d$ such that for all $k = 0, ..., N-1$ and $i = 1, ..., s$, c_d satisfies*

$$\begin{array}{ll} q_{k+1} = q_k + h \sum_{j=1}^s b_j V_k^j, & p_{k+1} = p_k + h \sum_{i=1}^s \hat{b}_j W_k^j, \\ Q_k^i = q_k + h \sum_{j=1}^s a_{ij} V_k^j, & P_k^i = p_k + h \sum_{j=1}^s \hat{a}_{ij} W_k^j, \\ W_k^i = D_1 L(Q_k^i, V_k^i) + f(Q_k^i, V_k^i), & P_k^i = D_2 L(Q_k^i, V_k^i), \end{array} \tag{4.9}$$

where the RK coefficients satisfy $b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j$ and $\hat{b}_i = b_i$.

Proof. That the curve $\boldsymbol{c}_d$ must restrict to the identities is clear from the fact that the discrete action, which is our discrete Lagrangian, satisfies

$$(\mathcal{J}_{\mathcal{HP}})_d [\hat{\imath} \boldsymbol{c}_d] = - (\mathcal{J}_{\mathcal{HP}})_d [\boldsymbol{c}_d] ;$$

therefore, the result from proposition 4.4.1 applies. A computation similar to that of theorem 3.2.4 leads to the equations (4.9) after restricting them to the identities with $q_{1,k} = q_{2,k} = q_k$, $p_{1,k} = p_{2,k} = p_k$, $Q_{1,k}^j = Q_{2,k}^j = Q_k^j$, $V_{1,k}^j = V_{2,k}^j = V_k^j$ and $P_{1,k}^j = P_{2,k}^j = P_k^j$ for all $k = 0, ..., N-1$ and $j = 1, ..., s$. □

Again, as with equations (4.10), if we define $\{v_k\}_{k=0}^N$ by the relation $p_k = D_2 L(q_k, v_k)$, we can rewrite the system in (4.9) as

$$\begin{aligned} q_{k+1} &= q_k + h \sum_{j=1}^s b_j V_k^j, \\ Q_k^i &= q_k + h \sum_{j=1}^s a_{ij} V_k^j, \\ D_2 L(q_{k+1}, v_{k+1}) &= D_2 L(q_k, v_k) + h \sum_{i=1}^s \hat{b}_j \left[D_1 L(Q_k^j, V_k^j) + f(Q_k^j, V_k^j) \right], \\ D_2 L(Q_k^i, V_k^i) &= D_2 L(q_k, v_k) + h \sum_{j=1}^s \hat{a}_{ij} \left[D_1 L(Q_k^j, V_k^j) + f(Q_k^j, V_k^j) \right] . \end{aligned} \tag{4.10}$$

4.4.2 Numerical tests

For our numerical tests we have chosen a well-known system composed of two coupled van der Pol oscillators [cf. Sch04, eq.(6.38)]. Remember that a single dimensionless van der Pol oscillator is described by the differential equation:

$$\ddot{q} - \left(\varepsilon - q^2\right) \dot{q} + q = 0$$

where ε is a parameter related to the damping of the system.

The dimensionless system we are going to study can be thought to be composed of two coupled harmonic oscillators with slightly differing natural frequencies under the action of non-linear forcing. Its configuration manifold is $\mathbb{T} \times \mathbb{T} = \mathbb{T}^2$, with velocity phase space

$T\mathbb{T}^2$, where we will use local coordinates (q_1, q_2, v_1, v_2), and the Lagrangian describing the non-forced part $L : T\mathbb{T}^2 \to \mathbb{R}$ is:

$$L = \frac{1}{2}\left(v_1^2 + v_2^2\right) - \frac{1}{2}\left[q_1^2 + (1+\rho)\, q_2^2\right] - \lambda\,(q_1 - q_2)^2$$

where ρ accounts for the deviation of q_2 from the natural frequency of q_1, and λ measures the intensity of the coupling between both oscillators. The van der Pol force acting on this system is $f = (\varepsilon - q_1^2)\, v_1 \mathrm{d}q_1 + (\varepsilon - q_2^2)\, v_2 \mathrm{d}q_2$. As our configuration space is flat, $\tau(q, Q) = Q - q$, and the generalized potential K is:

$$\boldsymbol{K}_f = \frac{1}{2}\sum_{i=1}^{2}\left[(\varepsilon - q_i^2)v_i + (\varepsilon - Q_i^2)V_i\right](q_i - Q_i)\ .$$

Note that for such an L and $\boldsymbol{K}_f$, at the identities we have that $v_i = p_i$, $i = 1, 2$, so they are interchangeable.

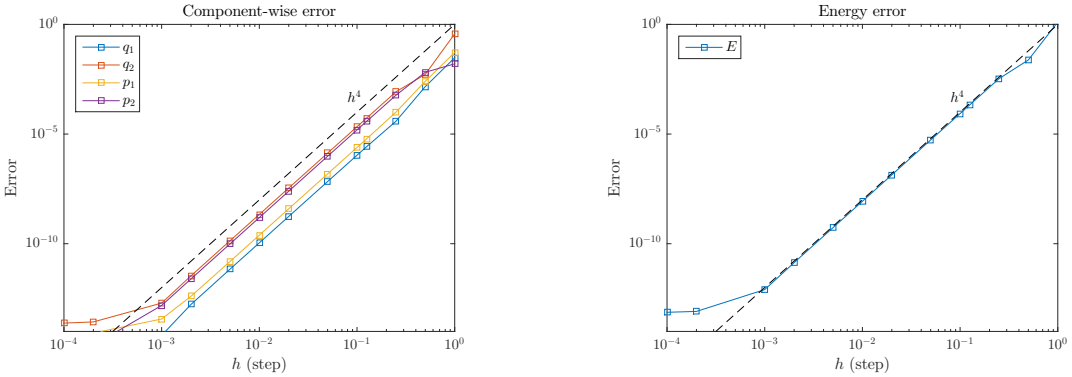


Figure 4.2: Numerical error on each separate component (left) and on the energy (right) for the Lobatto 3 method in a single simulation.

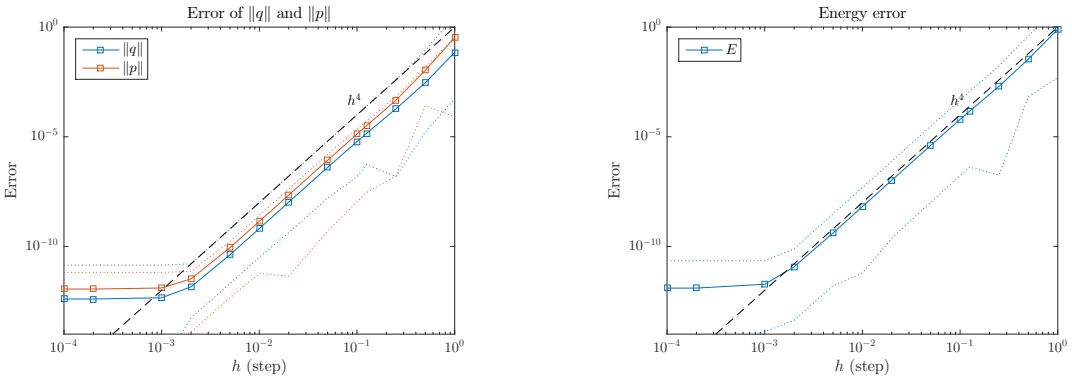


Figure 4.3: Numerical error of an ensemble for the Lobatto 3 method. Error in the norm of q and p (left) and on the energy (right). Dotted lines represent maximum and minimum of ensemble.

We chose to discretize the corresponding generalized Lagrangian, $\boldsymbol{L}_f$, using Lobatto schemes of 2, 3, 4 and 5 stages. The order of an s-stage Lobatto method is $p = 2s-2$ so the resulting numerical methods are of order 2, 4, 6 and 8 respectively. The parameters used for the numerical simulations shown here are $(\varepsilon, \rho, \lambda) = (0.5, 0.02, 0.8)$, for no particular

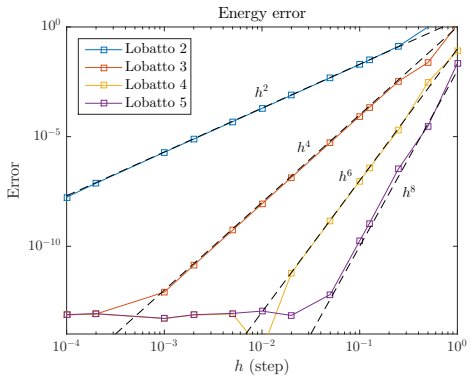


Figure 4.4: Errors in the energy for the different Lobatto methods.

reason. The other choices of parameters that were tested showed essentially the same behaviour. We ran each simulation for a total of 1 unit of simulation time with several different choices of step-size h ranging between $5 \cdot 10^{-5}$ and 1 and measured numerical error as the difference between the final value of the magnitude being studied found for a reference simulation and the corresponding one for the value we want to study. In this case our reference is taken as the simulation with the finest step-size. The initial values chosen for the results on diagrams 4.2 and 4.4 are $(q_1, q_2, v_1, v_2) = (-1/2, -1/4, 0, 4)$. The results shown on diagram 4.3 were found as the average from an ensemble of 25 random initial values in the square $[-4, 4] \times [-4, 4]$ and the pointed lines represent the maximum and minimum values found in said ensemble.

For the resolution of the resulting non-linear system of equations derived for each method, we used MATLAB's `fsolve` with `TolX=1e-12` and `TolX=1e-14`, which explains the flat tails.

Diagram 4.4 is a composite plot showing the error in the energy for the different Lobatto methods tested. The results are in agreement with the result of theorem 4.4.2. We have chosen to show only the energy to avoid clutter, but the same holds for each of the components of the system.

4.5 Mechanics and geometry of Galley's doubling in the reduced setting

In this section, we will study a purely variational description of the Euler-Poincaré and Lie-Poisson equations with forcing. We will see that the appropriate phase spaces for such Lagrangian and Hamiltonian mechanics are, respectively, $\mathfrak{g} \times G \times \mathfrak{g}$ and $\mathfrak{g}^* \times G \times \mathfrak{g}^*$.

In order to motivate the introduction of these spaces, it will be better to begin from the Lagrangian side, instead of diving directly into the geometric description.

4.5.1 Variational description of the forced Euler-Poincaré equations

First, consider a Lagrangian $\boldsymbol{L} : TG \times TG \to \mathbb{R}$ and the left-action $\Phi : G \times G \to G$, $\Phi_{g'}(g) = g'g = L_{g'}g$, and its tangent lift $\widehat{\Phi} : G \times TG \to TG$ given by

$$\widehat{\Phi}_{g'}(v_g) = T_g\Phi_{g'}(v_g) = g'v_g \in T_{g'g}G$$

and the corresponding diagonal action $\widehat{\Phi}^{\times}_{g'} : TG \times TG \to TG \times TG$ defined by:

$$\widehat{\Phi}^{\times}_{g'}(v_g, \tilde{v}_{\tilde{g}}) = (g' v_g, g' \tilde{v}_{\tilde{g}}) \,.$$

Assuming that $\boldsymbol{L}$ is $\widehat{\Phi}^{\times}$-invariant we deduce that

$$\boldsymbol{L}(v_g, \tilde{v}_{\tilde{g}}) = \boldsymbol{L}(g^{-1} v_g, g^{-1} \tilde{v}_{\tilde{g}}),$$

which lets us define the reduced Lagrangian $\boldsymbol{\ell} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$ by

$$\boldsymbol{\ell}(\eta, U, \psi) = \boldsymbol{L}(\eta, U\psi)$$

where $\eta = g^{-1} v_g, \psi = \tilde{g}^{-1} \tilde{v}_{\tilde{g}} \in \mathfrak{g}$ and $U = g^{-1}\tilde{g} \in G$.

We have the following

Theorem 4.5.1. *The Euler-Lagrange equations for $\boldsymbol{L}$ are equivalent to the reduced Euler-Lagrange equations for $\boldsymbol{\ell} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$:*

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{\ell}}{\partial \eta}\right) &= \mathrm{ad}^*_\eta \frac{\partial \boldsymbol{\ell}}{\partial \eta} - R^*_U \frac{\partial \boldsymbol{\ell}}{\partial U} \\ \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{\ell}}{\partial \psi}\right) &= \mathrm{ad}^*_\psi \frac{\partial \boldsymbol{\ell}}{\partial \psi} + L^*_U \frac{\partial \boldsymbol{\ell}}{\partial U} \\ \frac{\mathrm{d}U}{\mathrm{d}t} &= U\psi - \eta U \\ &= U(\psi - \mathrm{ad}_{U^{-1}}\eta) \,. \end{aligned} \tag{4.11}$$

Proof. Define the functional:

$$\mathcal{J}[(\eta, U, \psi)] = \int_0^T \boldsymbol{\ell}(\eta(t), U(t), \psi(t))\, dt$$

for some $T \in \mathbb{R} > 0$. Its critical points are the solutions of the corrresponding Euler-Lagrange equations. Taking variations

$$\mathrm{d}\mathcal{J}[(\eta, U, \psi)]((\delta\eta, \delta U, \delta\psi)) = \int_0^T \left[\frac{\partial \boldsymbol{\ell}}{\partial \eta}\delta\eta + \frac{\partial \boldsymbol{\ell}}{\partial U}\delta U + \frac{\partial \boldsymbol{\ell}}{\partial \psi}\delta\psi\right] dt = 0 \,.$$

We know that $\eta = g^{-1}\dot{g}$ and $\psi = \tilde{g}^{-1}\dot{\tilde{g}}$ and $U = g^{-1}\tilde{g}$. Therefore:

$$\begin{aligned} \delta\eta &= g^{-1}\delta\dot{g} - \Sigma\eta \\ \delta U &= U\widetilde{\Sigma} - \Sigma U \\ \delta\psi &= \tilde{g}^{-1}\delta\dot{\tilde{g}} - \widetilde{\Sigma}\psi \end{aligned}$$

where $\Sigma = g^{-1}\delta g$ and $\widetilde{\Sigma} = \tilde{g}^{-1}\delta\tilde{g}$. Also,

$$\begin{aligned} \dot{\Sigma} &= g^{-1}\delta\dot{g} - \eta\Sigma \\ \dot{\widetilde{\Sigma}} &= \tilde{g}^{-1}\delta\dot{\tilde{g}} - \psi\widetilde{\Sigma} \end{aligned}$$

and, in consequence,

$$\begin{aligned} \delta\eta &= [\eta, \Sigma] + \dot{\Sigma} \\ \delta U &= U\widetilde{\Sigma} - \Sigma U \\ \delta\psi &= [\psi, \widetilde{\Sigma}] + \dot{\widetilde{\Sigma}} \,. \end{aligned}$$

Since Σ and $\widetilde{\Sigma}$ are arbitrary, using integration by parts, we deduce the equations. □

A trivial example of such Lagrangians is given as follows. Consider a $\widehat{\Phi}$-invariant Lagrangian $L : TG \to \mathbb{R}$ with reduced Lagrangian $\ell : \mathfrak{g} \to \mathbb{R}$ and define a new Lagrangian $\boldsymbol{L} : TG \times TG \to \mathbb{R}$ as

$$\boldsymbol{L}(v_g, \tilde{v}_{\tilde{g}}) = L(\tilde{v}_{\tilde{g}}) - L(v_g).$$

Then, by (left-)trivialization we find that its associated reduced Lagrangian $\boldsymbol{\ell} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$ takes the form

$$\boldsymbol{\ell}(\eta, U, \psi) = \ell(\psi) - \ell(\eta).$$

According to the results of theorem 4.5.1, the equations of motion for this class of Lagrangians are simply two uncoupled and independent Euler-Poincaré equations.

A more general class of Lagrangians are those of the form

$$\boldsymbol{\ell}_{\boldsymbol{k}}(\eta, U, \psi) = \ell(\psi) - \ell(\eta) - \boldsymbol{k}(\eta, U, \psi),$$

where $\boldsymbol{k} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$ acts as a *generalized potential*. As it will become clear in the next section, if we still want to recuperate unique and clear dynamics on $\mathfrak{g}$, it will be crucial that these Lagrangians and potentials satisfy the discrete symmetry

$$\boldsymbol{k}(\psi, U^{-1}, \eta) = -\boldsymbol{k}(\eta, U, \psi),$$

which will result in two copies of the same dynamics when we restrict to initial conditions on the subset (η, e, η), that is, the restricted vector field they define projects onto $\mathfrak{g}$.

Our aim now is to obtain a generalized potential whose contribution to the dynamics on the aforementioned subset coincides with that of a given force, f. To do so, first consider the exponential map $\exp : \mathfrak{g} \to G$ (we choose exp but it is possible to take any other retraction map). Obviously, $\exp 0 = I$ and $T_0 \exp = \mathrm{Id}$ with the usual identifications. If we restrict ourselves to a neighborhood of the identity of the group, $\mathcal{U}_e$, then its inverse is well-defined.

With this we may then construct the function $\boldsymbol{k}_f : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$ by

$$\boldsymbol{k}_f(\eta, U, \psi) = \frac{1}{2}\left(\left\langle f(\psi), \exp^{-1} U^{-1}\right\rangle - \left\langle f(\eta), \exp^{-1} U\right\rangle\right)$$

where U is assumed to be in $\mathcal{U}_e$.

Proposition 4.5.1. *Let (ℓ, f) be a regular Lagrangian system with forcing given by $\ell : \mathfrak{g} \to \mathbb{R}$ and $f : \mathfrak{g} \to \mathfrak{g}^*$, and define the Lagrangian system $\boldsymbol{\ell}_f : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$ by*

$$\boldsymbol{\ell}_f(\eta, U, \psi) = \ell(\psi) - \ell(\eta) - \boldsymbol{k}_f(\eta, U, \psi).$$

Then we have that the following are equivalent:

- *$\sigma : I \subseteq \mathbb{R} \to \mathfrak{g}$ is a solution of the Euler-Poincaré equations with forcing*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta}\right) = \mathrm{ad}^*_\eta \frac{\partial \ell}{\partial \eta} + f(\eta)\,.$$

- *$\tilde{\sigma} : I \subseteq \mathbb{R} \to \mathfrak{g} \times G \times \mathfrak{g}$, that is, $\tilde{\sigma}(t) = (\sigma(t), e, \sigma(t))$ is a solution of the Euler-Lagrange equations for $\boldsymbol{\ell}_f$:*

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{\ell}_f}{\partial \eta}\right) - \mathrm{ad}^*_\eta \frac{\partial \boldsymbol{\ell}_f}{\partial \eta} + R^*_U \frac{\partial \boldsymbol{\ell}_f}{\partial U} = 0\\
&\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \boldsymbol{\ell}_f}{\partial \psi}\right) - \mathrm{ad}^*_\psi \frac{\partial \boldsymbol{\ell}_f}{\partial \psi} - L^*_U \frac{\partial \boldsymbol{\ell}_f}{\partial U} = 0\,.
\end{aligned}$$

Proof. Applying theorem 4.5.1 to $\boldsymbol{\ell}_f$ we get

$$-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \eta}-\frac{\partial \boldsymbol{k}_f}{\partial \eta}\right)+\mathrm{ad}^*_\eta\left(\frac{\partial \ell}{\partial \eta}-\frac{\partial \boldsymbol{k}_f}{\partial \eta}\right)-R^*_U\frac{\partial \boldsymbol{k}_f}{\partial U}=0$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \ell}{\partial \psi}-\frac{\partial \boldsymbol{k}_f}{\partial \psi}\right)-\mathrm{ad}^*_\psi\left(\frac{\partial \ell}{\partial \psi}-\frac{\partial \boldsymbol{k}_f}{\partial \psi}\right)+L^*_U\frac{\partial \boldsymbol{k}_f}{\partial U}=0\,.$$

Taking into account that $\exp^{-1}(e)=0$ and $T_e\exp^{-1}=\mathrm{Id}$, it is not difficult to see that on (η,e,η) the only surviving term from $\boldsymbol{k}_f$ is

$$\frac{\partial \boldsymbol{k}_f}{\partial U}(\eta,e,\eta)=-f(\eta).$$

Thus, on (η,e,η) the Euler-Lagrange equations for $\boldsymbol{\ell}_f$ reduce to two copies of the Euler-Poincaré equations with forcing, which proves our claim. □

4.5.2 Poisson groupoids

Throughout the rest of this chapter we will be working both with Lie groups and Lie groupoids. We will denote the latter by Γ and reserve G for the former to avoid confusion.

Definition 4.5.1. A **Poisson groupoid** is a Lie groupoid $\Gamma \rightrightarrows Q$, such that

1. $(\Gamma,\{\ ,\ \})$ is a Poisson manifold,
2. the graph of $\mu:\Gamma_2\to G$ is a coisotropic submanifold of $(\Gamma,-\{\ ,\ \})\times(\Gamma,-\{\ ,\ \})\times(\Gamma,\{\ ,\ \})$.

If Γ is a Poisson groupoid, then one may prove that [Wei88]

1. the identity section $\epsilon(Q)$ is coisotropic in Γ,
2. the inversion ι is an anti-Poisson morphism,
3. there is a unique Poisson structure on $\epsilon(Q)$ for which α is a Poisson mapping (and β is an anti-Poisson morphism).

We will be interested in a particular case of Poisson groupoids. Let G be a Lie group and $\mathfrak{g}$ its Lie algebra. The manifold $\Gamma\equiv\mathfrak{g}^*\times G\times\mathfrak{g}^*$ has a natural structure of a Lie groupoid where the structural maps are

$$\begin{aligned}\alpha(\lambda_1,U,\lambda_2)&=\lambda_1, & \iota(\lambda_1,U,\lambda_2)&=(\lambda_2,U,\lambda_1),\\ \beta(\lambda_1,U,\lambda_2)&=\lambda_2, & \epsilon(\lambda)&=(\lambda,e,\lambda),\\ \mu((\lambda_1,U,\lambda_2),(\lambda_2,V,\lambda_3))&=(\lambda_1,UV,\lambda_3),\end{aligned}\tag{4.12}$$

and the Poisson bracket is given by

$$\begin{aligned}\{\Xi_1,\Xi_2\}(\lambda_1,U,\lambda_2)&=0, & \{\Xi_1,F\}&=-\overrightarrow{\xi}F,\\ \{\Xi_1,\Xi_1'\}(\lambda_1,U,\lambda_2)&=\langle\lambda_1,[\xi,\xi']\rangle, & \{\Xi_2,F\}&=-\overleftarrow{\xi}F.\\ \{\Xi_2,\Xi_2'\}(\lambda_1,U,\lambda_2)&=-\langle\lambda_2,[\xi,\xi']\rangle,\end{aligned}\tag{4.13}$$

where $\xi, \xi' \in \mathfrak{g}$ induce the functions given by

$$\Xi_1(\lambda_1, U, \lambda_2) = \langle \lambda_1, \xi \rangle, \quad \Xi_1'(\lambda_1, U, \lambda_2) = \langle \lambda_1, \xi' \rangle,$$
$$\Xi_2(\lambda_1, U, \lambda_2) = \langle \lambda_2, \xi \rangle, \quad \Xi_2'(\lambda_1, U, \lambda_2) = \langle \lambda_2, \xi' \rangle,$$

and $F : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$ is the pull-back of a function on the Lie group G. The Lie groupoid $\mathfrak{g}^* \times G \times \mathfrak{g}^*$ equipped with this bracket is a Poisson groupoid. In some ocassions we will identify the function $\Xi_i \equiv \lambda_i$, $i = 1, 2$ when there is no possible confusion.

This linear Poisson bracket is completely determined by these functions. Still, for the sake of ease of computation, it may be helpful to have a more concrete expression. Let $A, B : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$, then their Poisson bracket can be written as

$$\begin{aligned}\{A, B\}(\lambda_1, U, \lambda_2) = &- \left\langle \lambda_2, \left[\frac{\partial A}{\partial \lambda_2}, \frac{\partial B}{\partial \lambda_2}\right] \right\rangle + \left\langle \lambda_1, \left[\frac{\partial A}{\partial \lambda_1}, \frac{\partial B}{\partial \lambda_1}\right] \right\rangle \\ &+ \left\langle L_U^* \frac{\partial A}{\partial U}, \frac{\partial B}{\partial \lambda_2} + \mathrm{Ad}_{U^{-1}} \frac{\partial B}{\partial \lambda_1} \right\rangle \\ &- \left\langle L_U^* \frac{\partial B}{\partial U}, \frac{\partial A}{\partial \lambda_2} + \mathrm{Ad}_{U^{-1}} \frac{\partial A}{\partial \lambda_1} \right\rangle.\end{aligned}$$

The following proposition is the Poisson analogue of proposition 4.3.2:

Proposition 4.5.2. *Let $\Gamma \rightrightarrows Q$ be a Poisson groupoid with Poisson bracket $\{\ ,\ \}$ and $E : \Gamma \to \mathbb{R}$ a function such that $E \circ \iota = -E$. Then, the corresponding Hamiltonian vector field X_E defined*

$$X_E(F) = \{F, E\},$$

verifies that $X_E(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q)$ for all $q \in Q$, and $F : \Gamma \to \mathbb{R}$.

Proof. We use that in a Poisson groupoid ι is a anti-Poisson morphism, that is,

$$\iota^* \left\{F, \tilde{F}\right\} = - \left\{\iota^* F, \iota^* \tilde{F}\right\},$$

for every $F, \tilde{F} : \Gamma \to \mathbb{R}$. This in particular implies that

$$T\iota(X_E) = -X_{E \circ \iota}$$

but since $E = -E \circ \iota$ then $T\iota(X_E) = X_E$. Now applying proposition 4.3.1 we deduce that $X_E(\epsilon(q)) \in T_{\epsilon(q)}\epsilon(Q)$. □

4.5.3 Free Hamiltonian description of the forced Lie-Poisson equations

Consider the Poisson groupoid $\mathfrak{g}^* \times G \times \mathfrak{g}^* \rightrightarrows \mathfrak{g}^*$ with the groupoid structure given by (4.12) and the linear Poisson structure (and associated Poisson bivector Π) defined by (4.13), and consider a Hamiltonian $\boldsymbol{\hbar} : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$.

If we denote an element of $\mathfrak{g}^* \times G \times \mathfrak{g}^*$ by (λ, U, μ), then the equations of motion defined by $\boldsymbol{\hbar}$ are the bracket equations

$$\begin{aligned} X_{\boldsymbol{\hbar}}(\lambda) &= \dot{\lambda} = \{\lambda, \boldsymbol{\hbar}\}, \\ X_{\boldsymbol{\hbar}}(\mu) &= \dot{\mu} = \{\mu, \boldsymbol{\hbar}\}, \\ X_{\boldsymbol{\hbar}}(U) &= \dot{\lambda} = \{U, \boldsymbol{\hbar}\}. \end{aligned}$$

Expanding these we get the Hamilton equations

$$\begin{aligned}\dot{\lambda} &= -\mathrm{ad}^*_{\partial\boldsymbol{\hbar}/\partial\lambda}\lambda - R^*_U\frac{\partial\boldsymbol{\hbar}}{\partial U}\\ \dot{\mu} &= \mathrm{ad}^*_{\partial\boldsymbol{\hbar}/\partial\mu}\mu - L^*_U\frac{\partial\boldsymbol{\hbar}}{\partial U}\\ \dot{U} &= U\left(\frac{\partial\boldsymbol{\hbar}}{\partial\mu} + \mathrm{Ad}_{U^{-1}}\frac{\partial\boldsymbol{\hbar}}{\partial\lambda}\right).\end{aligned} \tag{4.14}$$

Let us consider first a particular case of Hamiltonians on this groupoid.

Lemma 4.5.2. *Let $h : \mathfrak{g}^* \to \mathbb{R}$ be a Hamiltonian function. Consider the Hamiltonian $\boldsymbol{\hbar} : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$ defined by*

$$\boldsymbol{\hbar}(\lambda, U, \mu) = \hbar(\mu) - \hbar(\lambda)$$

then

1. *$\sharp^\Pi(\mathrm{d}\boldsymbol{\hbar}) = X_{\boldsymbol{\hbar}}$ is tangent to $\epsilon(\mathfrak{g}^*)$;*
2. *$X_{\boldsymbol{\hbar}}|_{\epsilon(\mathfrak{g}^*)} = \epsilon_*(X_\hbar)$.*

Proof. For the proof of the first part, observe that

$$(\boldsymbol{\hbar}\circ\iota)(\lambda, U, \mu) = \boldsymbol{\hbar}(\mu, U^{-1}, \lambda) = \hbar(\lambda) - \hbar(\mu) = -\boldsymbol{\hbar}(\lambda, U, \mu)$$

and apply proposition 4.5.2.

For the second part, it is easy to check using expressions (4.13) that

$$\begin{aligned}\{\Xi_1, \boldsymbol{\hbar}\}(\lambda, U, \mu) &= \left\langle \lambda, \left[\xi, \frac{\partial\boldsymbol{\hbar}}{\partial\lambda}\right]\right\rangle = -\left\langle \lambda, \left[\xi, \hbar'(\lambda)\right]\right\rangle\\ \{\Xi_2, \boldsymbol{\hbar}\}(\lambda, U, \mu) &= -\left\langle \mu, \left[\xi, \frac{\partial\boldsymbol{\hbar}}{\partial\mu}\right]\right\rangle = -\left\langle \mu, \left[\xi, \hbar'(\mu)\right]\right\rangle\\ \{F, \boldsymbol{\hbar}\}(\lambda, U, \mu) &= \left\langle L^*_U\frac{\partial F}{\partial U}, \frac{\partial\boldsymbol{\hbar}}{\partial\mu} + \mathrm{Ad}_{U^{-1}}\frac{\partial\boldsymbol{\hbar}}{\partial\lambda}\right\rangle\\ &= \left\langle L^*_U\frac{\partial F}{\partial U}, \hbar'(\mu) - \mathrm{Ad}_{U^{-1}}\hbar'(\lambda)\right\rangle\end{aligned}$$

where $F : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$ is the pull-back of a function on the Lie group G.

Therefore, if $F : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$ is the pull-back of a function on the Lie group G we have that

$$\begin{aligned}(X_{\boldsymbol{\hbar}})_{(\mu,e,\mu)}(\Xi_1) &= -\left\langle \mu, \left[\xi, \hbar'(\mu)\right]\right\rangle,\\ (X_{\boldsymbol{\hbar}})_{(\mu,e,\mu)}(\Xi_2) &= -\left\langle \mu, \left[\xi, \hbar'(\mu)\right]\right\rangle,\\ (X_{\boldsymbol{\hbar}})_{(\mu,e,\mu)}(F) &= 0,\end{aligned}$$

which is exactly the same as $\epsilon_*(X_\hbar)$ since

$$\epsilon_*(X_\hbar)(\mu, e, \mu) = \left(\mathrm{ad}^*_{\hbar'(\mu)}\mu, 0, \mathrm{ad}^*_{\hbar'(\mu)}\mu\right) \in \mathfrak{g}^* \times \mathfrak{g} \times \mathfrak{g}^* \equiv T_{(\mu,e,\mu)}(\mathfrak{g}^* \times G \times \mathfrak{g}^*).$$

□

Our aim is to generalize lemma 4.5.2 for the case of Lie-Poisson systems with forcing, that is, we have Hamiltonian function $\hbar : \mathfrak{g}^* \to \mathbb{R}$ and the force expressed by $\tilde{f} : \mathfrak{g}^* \to \mathfrak{g}^*$, both determining the Lie-Poisson equations with forcing

$$\dot{\mu} = \mathrm{ad}^*_{\hbar'(\mu)}\mu + \tilde{f}(\mu),$$

which define the vector field

$$Y_{\hbar,\tilde{f}}(\mu) = X_{\hbar}(\mu) + \sharp^{\Pi}(\tilde{f})(\mu) \in T_\mu\mathfrak{g}^* \equiv \mathfrak{g}^*. \tag{4.15}$$

Similar to the Lagrangian case let us define a function $\boldsymbol{k}_{\tilde{f}} : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$ by

$$\boldsymbol{k}_{\tilde{f}}(\lambda, U, \mu) = \frac{1}{2}\left(\left\langle \tilde{f}(\mu), \exp^{-1} U^{-1}\right\rangle - \left\langle \tilde{f}(\lambda), \exp^{-1} U\right\rangle\right)$$

where U is assumed to be in a neighborhood $\mathcal{U}_e$ of the identity element $e \in G$. With this we can state the following theorem.

Theorem 4.5.3. *Let $\hbar : \mathfrak{g}^* \to \mathbb{R}$ be a Hamiltonian function and $\tilde{f} : \mathfrak{g}^* \to \mathfrak{g}$ representing an external force. Consider the Hamiltonian $\boldsymbol{\hbar}_{\tilde{f}} : \mathfrak{g}^* \times G \times \mathfrak{g}^* \to \mathbb{R}$ defined by*

$$\boldsymbol{\hbar}_{\tilde{f}}(\lambda, U, \mu) = \hbar(\mu) - \hbar(\lambda) + \boldsymbol{k}_{\tilde{f}}(\lambda, U, \mu)$$

then

1. $\sharp^{\Pi}(\mathrm{d}\boldsymbol{\hbar}_{\tilde{f}}) = X_{\boldsymbol{\hbar}_{\tilde{f}}}$ *is tangent to* $\epsilon(\mathfrak{g}^*)$*;*
2. $X_{\boldsymbol{\hbar}_{\tilde{f}}}\Big|_{\epsilon(\mathfrak{g}^*)} = \epsilon_*\left(Y_{\hbar,\tilde{f}}\right)$.

Proof. The proof follows the same steps as those of lemma 4.5.2. For the first part observe that

$$\begin{aligned}(\boldsymbol{k}_{\tilde{f}} \circ \iota)(\lambda, U, \mu) &= \boldsymbol{k}_{\tilde{f}}(\mu, U^{-1}, \lambda)\\ &= \frac{1}{2}\left(\left\langle \tilde{f}(\lambda), \exp^{-1} U\right\rangle - \left\langle \tilde{f}(\mu), \exp^{-1} U^{-1}\right\rangle\right)\\ &= -\boldsymbol{k}_{\tilde{f}}(\lambda, U, \mu).\end{aligned}$$

For the second part, if one takes into account that $\exp^{-1}(e) = 0$ and $T_e\exp^{-1} = \mathrm{Id}$ then it is not difficult to see that

$$\begin{aligned}\left(X_{\boldsymbol{\hbar}_{\tilde{f}}}\right)_{(\mu,e,\mu)}(\Xi_1) &= -\left\langle \mu, \left[\xi, \hbar'(\mu)\right]\right\rangle + \left\langle \tilde{f}(\mu), \xi\right\rangle,\\ \left(X_{\boldsymbol{\hbar}_{\tilde{f}}}\right)_{(\mu,e,\mu)}(\Xi_2) &= -\left\langle \mu, \left[\xi, \hbar'(\mu)\right]\right\rangle + \left\langle \tilde{f}(\mu), \xi\right\rangle,\\ \left(X_{\boldsymbol{\hbar}_{\tilde{f}}}\right)_{(\mu,e,\mu)}(F) &= 0\,,\end{aligned}$$

which coincides with $\epsilon_*(Y_{\hbar,\tilde{f}})$. □

Proposition 4.5.3. *Let $(\hbar, \tilde{f})$ be a regular Hamiltonian system with forcing. Then its associated Hamiltonian $\boldsymbol{\hbar}_{\tilde{f}}$ is regular in a neighborhood of $\epsilon(\mathfrak{g}^*)$.*

Proof. Observe that the transformation

$$\begin{aligned}\mathbb{F}\boldsymbol{\hbar}^{\times}_{\tilde{f}}: \quad \mathfrak{g}^* \times G \times \mathfrak{g}^* &\to \mathfrak{g} \times G \times \mathfrak{g} \\ (\lambda, U, \mu) &\mapsto \left(-\tfrac{\partial \boldsymbol{\hbar}_{\tilde{f}}}{\partial \lambda}, U, \tfrac{\partial \boldsymbol{\hbar}_{\tilde{f}}}{\partial \mu}\right)\end{aligned}$$

reduces to $\mathbb{F}\boldsymbol{\hbar}^{\times}_{\tilde{f}}(\mu, e, \mu) = \left(\hbar'(\mu), e, \hbar'(\mu)\right)$ at the identity set. Then it must be a local diffeomorphism in a neighborhood of this set since its Hessian matrix

$$\begin{pmatrix} \hbar''(\mu) & 0 \\ 0 & \hbar''(\mu) \end{pmatrix}$$

is regular on $\epsilon(\mathfrak{g}^*)$ and therefore regular on a neighborhood of it. □

Relation with the Lagrangian formulation

Given a Lagrangian $\boldsymbol{\ell} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$, one may immediately define the usual fibre derivative $\mathbb{F}\boldsymbol{\ell}(\eta, g, \psi) = (\partial\boldsymbol{\ell}/\partial\eta, U, \partial\boldsymbol{\ell}/\partial\psi)$ to obtain a Hamiltonian description. However, in order to maintain the Poisson groupoid structure we have chosen, we can proceed as we did in the non-reduced case and define a modified fibre derivative:

$$\begin{aligned}\mathbb{F}\boldsymbol{\ell}^{\times}: \quad \mathfrak{g} \times G \times \mathfrak{g} &\to \mathfrak{g}^* \times G \times \mathfrak{g}^* \\ (\eta, U, \psi) &\mapsto \left(\lambda = -\tfrac{\partial \boldsymbol{\ell}}{\partial \eta}, U, \mu = \tfrac{\partial \boldsymbol{\ell}}{\partial \psi}\right),\end{aligned}$$

together with a modified interior product $\langle(\lambda, U, \mu), (\eta, U, \psi)\rangle_{\times} = \langle\mu, \psi\rangle - \langle\lambda, \eta\rangle$. One may quickly check that these definitions ensure that

$$\left\langle \mathbb{F}\boldsymbol{\ell}^{\times}(\eta, U, \psi), (\eta, U, \psi)\right\rangle_{\times} = \left\langle \mathbb{F}\boldsymbol{\ell}(\eta, U, \psi), (\eta, U, \psi)\right\rangle.$$

If the modified fibre derivative is a local diffeomorphism, then we may implicitly define the associated Hamiltonian by

$$\begin{aligned}\left(\boldsymbol{\hbar} \circ \mathbb{F}\boldsymbol{\ell}^{\times}\right)(\eta, U, \psi) &= E_{\boldsymbol{\ell}}(\eta, U, \psi) \\ &= \left\langle \mathbb{F}\boldsymbol{\ell}^{\times}(\eta, U, \psi), (\eta, U, \psi)\right\rangle_{\times} - \boldsymbol{\ell}(\eta, U, \psi).\end{aligned}$$

It is then a matter of simple computation to see that eqs.(4.11) and eqs.(4.14) are indeed equivalent.

Theorem 4.5.4. *Let (ℓ, f) and $(\hbar, \tilde{f})$ be a regular forced Lagrangian system and its associated forced Hamiltonian system, and denote by $\tilde{\boldsymbol{\hbar}}_{\tilde{f}} = E_{\boldsymbol{\ell}_f} \circ \left(\mathbb{F}\boldsymbol{\ell}^{\times}_f\right)^{-1}$ and $\boldsymbol{\hbar}_{\tilde{f}}$ the corresponding generalized Hamiltonians. Then their respective Hamiltonian vector fields $X_{\tilde{\boldsymbol{\hbar}}_{\tilde{f}}}$ and $X_{\boldsymbol{\hbar}_{\tilde{f}}}$ satisfy that $X_{\tilde{\boldsymbol{\hbar}}_{\tilde{f}}}\Big|_{\epsilon(\mathfrak{g}^*)} = X_{\boldsymbol{\hbar}_{\tilde{f}}}\Big|_{\epsilon(\mathfrak{g}^*)}$.*

Proof. As in theorem 4.5.3 we construct the extended Hamiltonian $\boldsymbol{\hbar}_{\tilde{f}}$, and we note that it coincides with the one implicitly defined as

$$\begin{aligned}\left(\boldsymbol{\hbar}_{\tilde{f}} \circ \mathbb{F}\boldsymbol{\ell}^{\times}\right)(\eta, U, \psi) &= E_{\boldsymbol{\ell}}(\eta, U, \psi) + \left(\tilde{\boldsymbol{k}} \circ \mathbb{F}\boldsymbol{\ell}^{\times}\right)(\eta, U, \psi) \\ &= \langle \ell'(\psi), \psi\rangle - \ell(\psi) - \langle \ell'(\eta), \eta\rangle + \ell(\eta) \\ &+ \frac{1}{2}\left(\left\langle f(\psi), \exp^{-1} U^{-1}\right\rangle - \left\langle f(-\eta), \exp^{-1} U\right\rangle\right),\end{aligned}$$

where $\boldsymbol{\ell}(\eta, U, \psi) = \ell(\psi) - \ell(\eta)$.

Applying the results of theorem 4.5.3 we have that

$$\left(\mathbb{F}\boldsymbol{\ell}^{\times}\right)^{*} \mathrm{d}\boldsymbol{\hbar}_{\tilde{f}}\big|_{\epsilon(\mathfrak{g})} = (-\eta, -f(\eta), \eta) \in \mathfrak{g} \times \mathfrak{g}^{*} \times \mathfrak{g}\,.$$

From the definition of the second Hamiltonian, $\tilde{\boldsymbol{\hbar}}_{\tilde{f}}$ and taking into account the results of proposition 4.5.3, it follows that

$$\left(\mathbb{F}\boldsymbol{\ell}_{f}^{\times}\right)^{*} \mathrm{d}\tilde{\boldsymbol{\hbar}}_{\tilde{f}}\Big|_{\epsilon(\mathfrak{g})} = (-\eta, -f(\eta), \eta),$$

and thus $\mathrm{d}\boldsymbol{\hbar}_{\tilde{f}}\big|_{\epsilon(\mathfrak{g}^{*})} = \mathrm{d}\tilde{\boldsymbol{\hbar}}_{\tilde{f}}\Big|_{\epsilon(\mathfrak{g}^{*})} = \Big(-\hbar'(\mu), -\tilde{f}(\mu), \hbar'(\mu)\Big)$, which together with the application of $\sharp^{\Pi}$ finishes our proof. □

4.6 Exact discrete Lagrangian in the forced reduced setting

4.6.1 Discrete variational description of the forced Euler-Poincaré equations

Consider a discrete Lagrangian $\boldsymbol{L}_d : G^4 = G \times G \times G \times G \to \mathbb{R}$ invariant under the action

$$\begin{array}{rccc} \widehat{\Phi}_d : & G \times G^4 & \longrightarrow & G^4 \\ & (g', (g_1, g_2, \tilde{g}_1, \tilde{g}_2)) & \longmapsto & (g'g_1, g'g_2, g'\tilde{g}_1, g'\tilde{g}_2) \end{array}$$

and define the reduced Lagrangian $\boldsymbol{\ell}_d : G \times G \times G \to \mathbb{R}$ by

$$\boldsymbol{\ell}_d(V, U, W) = \boldsymbol{L}_d(e, V, U, UW)$$

where $V = g_1^{-1}g_2$, $U = g_1^{-1}\tilde{g}_1$ and $W = \tilde{g}_1^{-1}\tilde{g}_2$.

Then, if $V_k = g_k^{-1}g_{k+1}$, $U_k = g_k^{-1}\tilde{g}_k$ and $W_k = \tilde{g}_k^{-1}\tilde{g}_{k+1}$, we have that

$$\begin{aligned} \delta V_k &= (L_{V_k})_{*}\mathrm{P}_{k+1} - (R_{V_k})_{*}\mathrm{P}_k, \\ \delta W_k &= (L_{W_k})_{*}\Sigma_{k+1} - (R_{W_k})_{*}\Sigma_k, \\ \delta U_k &= U_k\Sigma_k - \mathrm{P}_k U_k, \end{aligned}$$

where $\mathrm{P}_k = g_k^{-1}\delta g_k$ and $\Sigma_k = \tilde{g}_k^{-1}\delta\tilde{g}_k$.

Proposition 4.6.1. *Given a discrete Lagrangian $\boldsymbol{\ell}_d : G \times G \times G \to \mathbb{R}$, the following are equivalent:*

1. *The discrete variational principle*

$$\delta\mathcal{J}_d[c_d] = \sum_{i=0}^{N} \delta\boldsymbol{\ell}_d(V_k, U_k, W_k) = 0 \tag{4.16}$$

holds using variations of the form $\delta V_k = (L_{V_k})_{*}\mathrm{P}_{k+1} - (R_{V_k})_{*}\mathrm{P}_k$, $\delta W_k = (L_{W_k})_{*}\Sigma_{k+1} - (R_{W_k})_{*}\Sigma_k$ and $\delta U_k = U_k\Sigma_k - \mathrm{P}_k U_k$ where P_k, Σ_k are arbitrary with $\mathrm{P}_0, \Sigma_0, \mathrm{P}_N, \Sigma_N$ identically zero.

2. The discrete Euler-Lagrange equations hold:

$$\begin{aligned}(L_{V_{k-1}})^* D_1\boldsymbol{\ell}_d(V_{k-1},U_{k-1},W_{k-1}) =& (R_{V_k})^* D_1\boldsymbol{\ell}_d(V_k,U_k,W_k)\\ &+ (R_{U_k})^* D_2\boldsymbol{\ell}_d(V_k,U_k,W_k)\\ (L_{W_{k-1}})^* D_3\boldsymbol{\ell}_d(V_{k-1},U_{k-1},W_{k-1}) =& (R_{W_k})^* D_3\boldsymbol{\ell}_d(V_k,U_k,W_k)\\ &- (L_{U_k})^* D_2\boldsymbol{\ell}_d(V_k,U_k,W_k)\\ U_k =& V_{k-1}^{-1}U_{k-1}W_{k-1}\,.\end{aligned} \tag{4.17}$$

Proof. The last equation is a consequence of the definitions. The remaining two equations follow from a straightforward computation of the variations and rearrangement of the terms of the sum. [See also MMM06, for the general case of Lie groupoids.] □

These equations are the discrete equivalent of the equations given in theorem 4.5.1, and under certain regularity conditions they define a discrete flow [see MMM06],

$$F_{\boldsymbol{\ell}_d}(V_{k-1},U_{k-1},W_{k-1}) = (V_k,U_k,W_k).$$

Much like in the standard setting, in this reduced setting we can define two discrete Legendre transformations

$$\mathbb{F}^{\pm}\boldsymbol{\ell}_d^{\times} : G\times G\times G \to \mathfrak{g}^*\times G\times\mathfrak{g}^*$$

with coordinate presentation

$$\begin{aligned}\mathbb{F}^{+}\boldsymbol{\ell}_d^{\times}(V_k,U_k,W_k) = (&-(L_{V_k})^* D_1\boldsymbol{\ell}_d(V_k,U_k,W_k),\\ &V_k^{-1}U_kW_k,\\ &(L_{W_k})^* D_3\boldsymbol{\ell}_d(V_k,U_k,W_k))\\ \mathbb{F}^{-}\boldsymbol{\ell}_d^{\times}(V_k,U_k,W_k) = (&-(R_{V_k})^* D_1\boldsymbol{\ell}_d(V_k,U_k,W_k) - (R_{U_k})^* D_2\boldsymbol{\ell}_d(V_k,U_k,W_k),\\ &U_k,\\ &(R_{W_k})^* D_3\boldsymbol{\ell}_d(V_k,U_k,W_k) - (L_{U_k})^* D_2\boldsymbol{\ell}_d(V_k,U_k,W_k))\,.\end{aligned}$$

4.6.2 The exact discrete Lagrangian

Given a regular Lagrangian function $\boldsymbol{\ell} : \mathfrak{g}\times G\times\mathfrak{g} \longrightarrow \mathbb{R}$, we will consider discrete Lagrangians $\boldsymbol{\ell}_d$ as an approximation to the action of the continuous Lagrangian which can be considered as the exact discrete Lagrangian:

$$\boldsymbol{\ell}_d^e(V_0,U_0,W_0,h) = \int_0^h \boldsymbol{\ell}(\eta(t),U(t),\psi(t))\mathrm{d}t,$$

where $t\to(\eta(t),U(t),\psi(t))$ is the unique solution of the Euler-Lagrange equations for $\boldsymbol{\ell}$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\boldsymbol{\ell}}{\partial\eta}\right) &= \mathrm{ad}^*_\eta\frac{\partial\boldsymbol{\ell}}{\partial\eta} - R^*_U\frac{\partial\boldsymbol{\ell}}{\partial U}\\ \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\boldsymbol{\ell}}{\partial\psi}\right) &= \mathrm{ad}^*_\psi\frac{\partial\boldsymbol{\ell}}{\partial\psi} + L^*_U\frac{\partial\boldsymbol{\ell}}{\partial U}\\ \dot{U} &= U(\psi-\mathrm{ad}_{U^{-1}}\eta)\end{aligned}$$

together with the reconstruction equations:

$$\dot{g}(t) = g(t)\eta(t)$$
$$\dot{\tilde{g}}(t) = \tilde{g}(t)\psi(t)$$

satisfying $g(0) = e$, $g(h) = V_0$, $\tilde{g}(0) = U_0$ and $\tilde{g}(h) = U_0W_0$ with small enough h [see MMM16].

As usual, we say $\boldsymbol{\ell}_d(V_0, U_0, W_0, h)$ is an *approximation of order* r (to the exact discrete Lagrangian) if there exists an open subset $\mathcal{U}_s \subset G \times \mathfrak{g} \times G \times \mathfrak{g}$ with compact closure and constants C_s and h_s such that

$$\|\boldsymbol{\ell}_d(V(h), U_0, W(h), h) - \boldsymbol{\ell}_d^e(V(h), U_0, W(h), h)\| \leq C_s h^{r+1},$$

with $V(h) = g^{-1}(0)g(h)$, $W(h) = \tilde{g}^{-1}(0)\tilde{g}(h)$ and $U_0 = g^{-1}(0)\tilde{g}(0)$, for all solutions $(g(t), \eta(t), \tilde{g}(t), \psi(t))$ of the Euler-Lagrange equations with initial condition in $\mathcal{U}_s$ and for all $h \leq h_s$.

As is common practice, we will fix some h and drop its explicit dependence unless it is strictly necessary.

In previous sections we considered Lagrangians $\boldsymbol{L} : TG \times TG \to \mathbb{R}$ and their reduced counterparts $\boldsymbol{\ell} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$, which displayed discrete symmetries of the form $\boldsymbol{L}(\tilde{v}_{\tilde{g}}, v_g) = -\boldsymbol{L}(v_g, \tilde{v}_{\tilde{g}})$ and $\boldsymbol{\ell}(\eta, U, \psi) = -\boldsymbol{\ell}(\psi, U^{-1}, \eta)$ and we saw the groupoidal interpretation of this operation (on the Hamiltonian side).

In the discrete realm we may define an equivalent transformation $\iota_d : G^4 \to G^4$ and its induced transformation $\check{\iota}_d : G \times G \times G \to G \times G \times G$,

$$\iota_d(g_1, g_2, \tilde{g}_1, \tilde{g}_2) = (\tilde{g}_1, \tilde{g}_2, g_1, g_2)$$
$$\check{\iota}_d(V, U, W) = (W, U^{-1}, V)\,.$$

We can state the following trivial proposition.

Proposition 4.6.2. *Let $\boldsymbol{\ell} : \mathfrak{g} \times G \times \mathfrak{g} \to \mathbb{R}$ be a Lagrangian satisfying that $\boldsymbol{\ell}(\psi, U^{-1}, \eta) = -\boldsymbol{\ell}(\eta, U, \psi)$ for all $(\eta, U, \psi) \in \mathfrak{g} \times G \times \mathfrak{g}$. Then its exact discrete Lagrangian, $\boldsymbol{\ell}_d^e : G \times G \times G \to \mathbb{R}$ satisfies $\boldsymbol{\ell}_d^e \circ \check{\iota}_d = -\boldsymbol{\ell}_d^e$.*

It is always possible to work with approximations of $\boldsymbol{\ell}_d^e$ that respect this symmetry, that is, $\boldsymbol{\ell}_d \approx \boldsymbol{\ell}_d^e$ satisfying $\boldsymbol{\ell}_d \circ \check{\iota}_d = -\boldsymbol{\ell}_d$. Such discrete Lagrangians will be of crucial importance to derive variationally forced integrators.

If we define the maps $\epsilon_d : G \times G \to G^4$ and $\check{\epsilon}_d : G \to G \times G \times G$ by

$$\epsilon_d(g_1, g_2) = (g_1, g_2, g_1, g_2),$$
$$\check{\epsilon}_d(V) = (V, e, V),$$

respectively, then we can prove the following

Theorem 4.6.1. *The discrete flow $F_{\boldsymbol{\ell}_d} : G \times G \times G \to G \times G \times G$ defined by a discrete Lagrangian $\boldsymbol{\ell}_d : G \times G \times G \to \mathbb{R}$ verifying that $\boldsymbol{\ell}_d \circ \check{\iota}_d = -\boldsymbol{\ell}_d$ restricts to $\check{\epsilon}_d(G)$, that is,*

$$F_{\boldsymbol{\ell}_d} \circ \check{\epsilon}_d(G) \in \check{\epsilon}_d(G).$$

Proof. If we apply the identity $\boldsymbol{\ell}_d \circ \check{\iota}_d = -\boldsymbol{\ell}_d$ to

$$\sum_{i=0}^{N} \left(\boldsymbol{\ell}_d \circ \check{\iota}_d\right)(V_k, U_k, W_k) \tag{4.18}$$

and apply the discrete Hamilton principle we obtain eq.(4.16), and it follows immediately that solutions of the system

$$\begin{aligned}
(L_{W_{k-1}})^* D_1\boldsymbol{\ell}_d(W_{k-1}, U_{k-1}^{-1}, V_{k-1}) &= (R_{W_k})^* D_1\boldsymbol{\ell}_d(W_k, U_k^{-1}, V_k) \\
&\quad + (R_{U_k^{-1}})^* D_2\boldsymbol{\ell}_d(W_k, U_k^{-1}, V_k), \\
(L_{V_{k-1}})^* D_3\boldsymbol{\ell}_d(W_{k-1}, U_{k-1}^{-1}, V_{k-1}) &= (R_{V_k})^* D_3\boldsymbol{\ell}_d(W_k, U_k^{-1}, V_k) \\
&\quad - (L_{U_k^{-1}})^* D_2\boldsymbol{\ell}_d(W_k, U_k^{-1}, V_k), \\
U_k^{-1} &= W_{k-1}^{-1} U_{k-1}^{-1} V_{k-1},
\end{aligned}$$

obtained from varying eq.(4.18) must also be solutions of eqs.(4.17). If we restrict either these or eqs.(4.17) to $\check{\epsilon}_d(G)$, the last equation turns into an identity and the remaining equations become

$$\begin{aligned}
(L_{V_{k-1}})^* D_1\boldsymbol{\ell}_d(V_{k-1}, e, V_{k-1}) &= (R_{V_k})^* D_1\boldsymbol{\ell}_d(V_k, e, V_k) + D_2\boldsymbol{\ell}_d(V_k, e, V_k), \\
(L_{V_{k-1}})^* D_3\boldsymbol{\ell}_d(V_{k-1}, e, V_{k-1}) &= (R_{V_k})^* D_3\boldsymbol{\ell}_d(V_k, e, V_k) - D_2\boldsymbol{\ell}_d(V_k, e, V_k).
\end{aligned}$$

The vanishing of the dynamics in U_k proves that $F_{\boldsymbol{\ell}_d}|_{\check{\epsilon}_d(G)} : \check{\epsilon}_d(G) \to \check{\epsilon}_d(G)$. □

Theorem 4.6.2. *Let (L, F) be a $\widehat{\Phi}^{\times}$-invariant forced regular Lagrangian system in G such that it defines an (l, f) forced regular Lagrangian system in $\mathfrak{g}$. Denote by $\boldsymbol{L}_F : TG \times TG \to \mathbb{R}$ the extended Lagrangian, and let $\boldsymbol{L}_{F,d} : G^4 \to \mathbb{R}$ be a $\widehat{\Phi}_d$-invariant approximation to the exact discrete Lagrangian of order r satisfying $\boldsymbol{L}_{F,d} \circ \iota_d = -\boldsymbol{L}_{F,d}$. Then,*

- *The discrete Lagrangian $\boldsymbol{\ell}_{f,d} : G \times G \times G \to \mathbb{R}$ defined by*

  $$\boldsymbol{\ell}_{f,d}(V, U, W) = \boldsymbol{L}_{F,d}(e, V, U, UW),$$

  is an approximation of order r for $\boldsymbol{\ell}^e_{f,d}$ satisfying the identity $\boldsymbol{\ell}_{f,d} \circ \check{\iota}_d = -\boldsymbol{\ell}_{f,d}$.

- *When restricted to $\epsilon_d(G \times G)$, the discrete flow $F_{\boldsymbol{L}_{F,d}} : G^4 \to G^4$ induced by its discrete Euler-Lagrange equations is an approximation of order r to the flow of (L, F).*

- *When restricted to $\check{\epsilon}_d(G)$, the discrete flow $F_{\boldsymbol{\ell}_{f,d}} : G \times G \times G \to G \times G \times G$ induced by its discrete Euler-Lagrange equations is an approximation of order r to the flow of (l, f).*

Proof. We have that for h sufficiently small

$$\begin{aligned}
\boldsymbol{L}_{F,d}(g_0, g_1, \tilde{g}_0, \tilde{g}_1) &= \boldsymbol{L}^e_{F,d}(g_0, g_1, \tilde{g}_0, \tilde{g}_1) + \mathcal{O}\left(h^{r+1}\right) \\
&= \int_0^h \boldsymbol{L}_F(g(t), \dot{g}(t), \tilde{g}(t), \dot{\tilde{g}}(t))\mathrm{d}t + \mathcal{O}\left(h^{r+1}\right),
\end{aligned}$$

where $(g(t), \dot{g}(t), h(t), \dot{h}(t))$ is a solution of the Euler-Lagrange equations for $\boldsymbol{L}_F$ such that $g(0) = g_0 = e$, $g(h) = g_1$, $\tilde{g}(0) = \tilde{g}_0$, $\tilde{g}(h) = \tilde{g}_1$. This means that, by $\widehat{\Phi}^{\times}$-invariance,

$$\boldsymbol{L}_{F,d}(g_0, g_1, \tilde{g}_0, \tilde{g}_1) = \int_0^h \boldsymbol{\ell}_F(\eta(t), U(t), \psi(t))\mathrm{d}t + \mathcal{O}\left(h^{r+1}\right),$$

with $\eta(t) = g^{-1}(t)\dot{g}(t)$, $U(t) = g^{-1}(t)h(t)$ and $\psi(t) = h^{-1}(t)\dot{h}(t)$ and by $\widehat{\Phi}_d$-invariance we get

$$\boldsymbol{L}_{F,d}(g_0, g_1, \tilde{g}_0, \tilde{g}_1) = \boldsymbol{L}_{F,d}(e, g_0^{-1}g_1, g_0^{-1}\tilde{g}_0, g_0^{-1}\tilde{g}_1) = \boldsymbol{\ell}_{f,d}(V_0, U_0, W_0),$$

with $V_0 = g_0^{-1}g_1$, $U_0 = g_0^{-1}\tilde{g}_0$, $W_0 = \tilde{g}_0^{-1}\tilde{g}_1$. Thus $\boldsymbol{\ell}_{f,d}$ is indeed of order r with respect to $\boldsymbol{\ell}^e_{f,d}$.

That $\boldsymbol{\ell}_{f,d}$ satisfies $\boldsymbol{\ell}_{f,d} \circ \check{\iota}_d = -\boldsymbol{\ell}_{f,d}$ follows immediately from its definition from $\boldsymbol{L}_{F,d}$, i.e.

$$\begin{aligned}(\boldsymbol{\ell}_{f,d} \circ \check{\iota}_d)(V_0, U_0, W_0) &= (\boldsymbol{L}_{F,d} \circ \iota_d)(g_0, g_1, \tilde{g}_0, \tilde{g}_1)\\ &= -\boldsymbol{L}_{F,d}(\tilde{g}_0, \tilde{g}_1, g_0, g_1),\\ &= -\boldsymbol{L}_{F,d}(e, \tilde{g}_0^{-1}\tilde{g}_1, \tilde{g}_0^{-1}g_0, \tilde{g}_0^{-1}g_1),\\ &= -\boldsymbol{\ell}_{f,d}(W_0, U_0^{-1}, V_0).\end{aligned}$$

In the second point it suffices to apply the variational error theorem from [PC09], which proves that $F_{\boldsymbol{L}_{F,d}}$ is an approximation of order r to the exact Hamiltonian flow induced by the Euler-Lagrange equations. Afterwards, we only need to apply theorem 4.6.1 to see that the discrete flow projects onto G, thus approximating the continuous flow for the forced Lagrangian system (L, F).

The third point can then be seen as a direct consequence of the second point. If $\check{\pi}_d : G^4 \to G^4/G \equiv G \times G \times G$, then it is clear that $\check{\pi}_d \circ F_{\boldsymbol{L}^h_{F,d}} = F_{\boldsymbol{\ell}^h_{f,d}} \circ \check{\pi}_d$, and $\check{\pi}_d$ does not affect the order, so the result follows immediately. □

Remark. This theorem can be proven without mentioning the forced system (L, F) or the discrete Lagrangian $\boldsymbol{L}_{F,d}$ at all, by directly applying the results of [MMM16, theorem 5.7 in particular] and then applying theorem 4.6.1. △

4.6.3 Variationally partitioned Runge-Kutta-Munthe-Kaas methods with forcing

For an introduction to these methods, please check section 3.4.

If we consider the pair groupoid $TG \times TG$ with local coordinates $(g, \dot{g}, \widetilde{g}, \dot{\widetilde{g}})$, a regular Lagrangian $\boldsymbol{L} : TG \times TG \to \mathbb{R}$, and a quadrature rule associated to the RK method we want to apply, an approximation to the exact discrete Lagrangian can be written as

$$\boldsymbol{L}_d(g_0, g_N, \widetilde{g}_0, \widetilde{g}_N) = \sum_{k=0}^{N-1} \boldsymbol{L}_d(g_k, g_{k+1}, \widetilde{g}_k, \widetilde{g}_{k+1}) = \sum_{k=0}^{N-1}\sum_{i=1}^{s} b_i h \boldsymbol{L}(G_k^i, \dot{G}_k^i, \widetilde{G}_k^i, \dot{\widetilde{G}}_k^i)$$

where

$$\begin{aligned}G_k^i &= g_k \tau\left(\Xi_k^i\right),\\ \dot{G}_k^i &= g_k \tau\left(\Xi_k^i\right) \mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i,\\ \widetilde{G}_k^i &= \tilde{g}_k \tau\left(\mathrm{X}_k^i\right),\\ \dot{\widetilde{G}}_k^i &= \tilde{g}_k \tau\left(\mathrm{X}_k^i\right) \mathrm{d}^L \tau_{\mathrm{X}_k^i} \Psi_k^i,\end{aligned}$$

and $(\Xi_k^i, \mathrm{H}_k^i, \mathrm{X}_k^i, \Psi_k^i) \in T\mathfrak{g} \times T\mathfrak{g}$ are chosen so as to extremize the discrete action subject to the constraints

$$\begin{aligned}
\Xi_k^i &= h \sum_{j=1}^{s} a_{ij} \mathrm{H}_k^j, \\
\tau^{-1}((g_k)^{-1} g_{k+1}) = \xi_{k,k+1} &= h \sum_{j=1}^{s} b_j \mathrm{H}_k^j \\
\mathrm{X}_k^i &= h \sum_{j=1}^{s} a_{ij} \Psi_k^j, \\
\tau^{-1}((\widetilde{g}_k)^{-1} \widetilde{g}_{k+1}) = \chi_{k,k+1} &= h \sum_{j=1}^{s} b_j \Psi_k^j.
\end{aligned}$$

If $\boldsymbol{L}$ is $\widehat{\Phi}^{\times}$-invariant, then the discrete Lagrangian can be rewritten as

$$\begin{aligned}
\boldsymbol{L}_d(g_k, g_{k+1}, \widetilde{g}_k, \widetilde{g}_{k+1}) &= h \sum_{i=1}^{s} b_i \boldsymbol{\ell}(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i, \tau(-\Xi_k^i) g_k^{-1} \widetilde{g}_k \tau(\mathrm{X}_k^i), \mathrm{d}^L \tau_{\mathrm{X}_k^i} \Psi_k^i) \\
&= \boldsymbol{\ell}_d(V_k \equiv g_k^{-1} g_{k+1}, U_k \equiv g_k^{-1} \widetilde{g}_k, W_k \equiv \widetilde{g}_k^{-1} \widetilde{g}_{k+1}).
\end{aligned}$$

The equations resulting from the extremization process are

$$\begin{aligned}
\lambda_{k+1} &= \mathrm{Ad}^*_{\xi_{k,k+1}} \left[\lambda_k + h \sum_{j=1}^{s} b_j R^*_{U_k} \widehat{\mathrm{K}}_k^i \right] \\
\mu_{k+1} &= \mathrm{Ad}^*_{\chi_{k,k+1}} \left[\mu_k + h \sum_{j=1}^{s} b_j L^*_{U_k} \widehat{\mathrm{K}}_k^i \right] \\
\Lambda_k^i &= \mathrm{Ad}^*_{\xi_{k,k+1}} \left[\lambda_k + h \sum_{j=1}^{s} b_j \left(R^*_{U_k} \widehat{\mathrm{K}}_k^j - \frac{a_{ji}}{b_i} \left(\mathrm{d}^L \tau_{\Xi_k^j} \mathrm{d}^L \tau^{-1}_{-\xi_{k,k+1}} \right)^* R^*_{\tau(-\Xi_k^j) U_k \tau(\mathrm{X}_k^j)} \mathrm{K}_k^j \right) \right] \\
\mathrm{M}_k^i &= \mathrm{Ad}^*_{\chi_{k,k+1}} \left[\mu_k + h \sum_{j=1}^{s} b_j \left(L^*_{U_k} \widehat{\mathrm{K}}_k^j - \frac{a_{ji}}{b_i} \left(\mathrm{d}^L \tau_{\mathrm{X}_k^j} \mathrm{d}^L \tau^{-1}_{-\chi_{k,k+1}} \right)^* L^*_{\tau(-\Xi_k^j) U_k \tau(\mathrm{X}_k^j)} \mathrm{K}_k^j \right) \right]
\end{aligned}$$

where

$$\begin{aligned}
\lambda_k &= -D_1 \boldsymbol{\ell}(\eta_k, U_k, \psi_k) \\
\mu_k &= D_3 \boldsymbol{\ell}(\eta_k, U_k, \psi_k) \\
\Pi_k^i &= -\left(\mathrm{d}^L \tau_{\Xi_k^i} \right)^* D_1 \boldsymbol{\ell}(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i, \tau(-\Xi_k^i) U_k \tau(\mathrm{X}_k^i), \mathrm{d}^L \tau_{\mathrm{X}_k^i} \Psi_k^i)) \\
\mathrm{P}_k^i &= \left(\mathrm{d}^L \tau_{\mathrm{X}_k^i} \right)^* D_3 \boldsymbol{\ell}(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i, \tau(-\Xi_k^i) U_k \tau(\mathrm{X}_k^i), \mathrm{d}^L \tau_{\mathrm{X}_k^i} \Psi_k^i)) \\
\Lambda_k^i &= \left(\mathrm{d}^L \tau^{-1}_{\xi_{k,k+1}} \right)^* \left[\Pi_k^i + h \sum_{j=1}^{s} \frac{b_j a_{ji}}{b_i} \left(\mathrm{dd}^L \tau^{-1}_{\Xi_k^j} \right)^* (\mathrm{H}_k^j, \Pi_k^j) \right] \\
\mathrm{M}_k^i &= \left(\mathrm{d}^L \tau^{-1}_{\chi_{k,k+1}} \right)^* \left[\mathrm{P}_k^i + h \sum_{j=1}^{s} \frac{b_j a_{ji}}{b_i} \left(\mathrm{dd}^L \tau^{-1}_{\mathrm{X}_k^j} \right)^* (\Psi_k^j, \mathrm{P}_k^j) \right] \\
\mathrm{K}_k^i &= D_2 \boldsymbol{\ell}(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i, \tau(-\Xi_k^i) U_k \tau(\mathrm{X}_k^i), \mathrm{d}^L \tau_{\mathrm{X}_k^i} \Psi_k^i)) \\
\widehat{\mathrm{K}}_k^i &= L^*_{\tau(-\Xi_k^i)} R^*_{\tau(\mathrm{X}_k^i)} \mathrm{K}_k^i \,.
\end{aligned}$$

Note that $V_k = \tau(\xi_{k,k+1})$ and $W_k = \tau(\chi_{k,k+1})$, so we can write

$$U_{k+1} = \tau(-\xi_{k,k+1}) U_k \tau(\chi_{k,k+1}).$$

Restriction to the identities in this setting means $\Xi_k^i = \mathrm{X}_k^i$, $\xi_{k,k+1} = \chi_{k,k+1}$, $\mathrm{H}_k^i = \Psi_k^i$, $\lambda_k = \mu_k$, $\Lambda_k^i = \mathrm{M}_k^i$ and $U_k = e$. For a Lagrangian $\boldsymbol{\ell}_f$, when we restrict these equations to the identities we find that

$$\begin{aligned}
\lambda_k &= \ell'(\eta_k) \\
\Pi_k^i &= \left(\mathrm{d}^L \tau_{\Xi_k^i}\right)^* \ell'(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i) \\
\mathrm{K}_k^i &= f(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i) \\
\widehat{\mathrm{K}}_k^i &= \left(\mathrm{Ad}^{-1}_{\tau(\Xi_k^i)}\right)^* f(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i).
\end{aligned}$$

It is convenient to define

$$\mathrm{N}_k^i = \left(\mathrm{d}^L \tau_{\Xi_k^i}\right)^* f(\mathrm{d}^L \tau_{\Xi_k^i} \mathrm{H}_k^i),$$

which, taking into account that $\mathrm{Ad}^{-1}_{\tau(\xi)} = \mathrm{d}^L \tau_\xi \mathrm{d}^L \tau^{-1}_{-\xi}$, allows us to write

$$\widehat{\mathrm{K}}_k^i = \left(\mathrm{d}^L \tau^{-1}_{-\Xi_k^i}\right)^* \mathrm{N}_k^i.$$

This lets us rewrite the equations at the identities as

$$\begin{aligned}
\lambda_{k+1} &= \mathrm{Ad}^*_{\xi_{k,k+1}} \left[\lambda_k + h \sum_{j=1}^s b_j \left(\mathrm{d}^L \tau^{-1}_{-\Xi_k^j}\right)^* \mathrm{N}_k^j \right] \\
\Lambda_k^i &= \mathrm{Ad}^*_{\xi_{k,k+1}} \left[\lambda_k + h \sum_{j=1}^s b_j \left(\mathrm{d}^L \tau^{-1}_{-\Xi_k^j} - \frac{a_{ji}}{b_i} \mathrm{d}^L \tau^{-1}_{-\xi_{k,k+1}} \right)^* \mathrm{N}_k^j \right],
\end{aligned}$$

which is precisely the form the variationally partitioned RKMK equations were expected to take for a reduced Lagrangian with forcing.

4.6.4 Numerical tests

For our numerical tests we have chosen a simplified version of the Landau-Lifschitz-Gilbert (LLG) model for ferromagnetic materials [Lan67, art. 18].

The configuration manifold of the system is the Lie group $SO(3)$, whose Lie algebra is $\mathfrak{so}(3) \cong \mathbb{R}^3$. Its velocity phase space is therefore $TSO(3) \equiv SO(3) \times \mathbb{R}^3$. Its Lagrangian $L : TSO(3) \to \mathbb{R}$ is just the standard rigid body Lagrangian, which is invariant under the action of the group; therefore, we may work with the following reduced Lagrangian $\ell : \mathbb{R}^3 \to \mathbb{R}$

$$\ell(\boldsymbol{\Omega}) = \frac{1}{2} \boldsymbol{\Omega}^T I \boldsymbol{\Omega}$$

where I denotes here the inertia tensor of the particle and $\boldsymbol{\Omega} \in \mathbb{R}^3$, with coordinates $(\Omega_x, \Omega_y, \Omega_z)$.

The Euler-Poincaré equations for this simple Lagrangian are the well-known Euler equations for the rigid body,

$$\dot{\mathbf{M}} = \mathbf{M} \times \boldsymbol{\Omega}$$

where $\frac{\partial \ell}{\partial \boldsymbol{\Omega}} = \mathbf{M} = I\boldsymbol{\Omega}$ and $\mathrm{ad}^*_{\boldsymbol{\Omega}} \frac{\partial \ell}{\partial \boldsymbol{\Omega}} = \mathbf{M} \times \boldsymbol{\Omega}$.

The simplified LLG force is of the form

$$f = \alpha \mathbf{M} \times (\mathbf{M} \times \boldsymbol{\Omega})$$

with $\alpha \in \mathbb{R}$ a constant. Therefore, the equations of motion are

$$\dot{\mathbf{M}} = \mathbf{M} \times \boldsymbol{\Omega} + \alpha \mathbf{M} \times (\mathbf{M} \times \boldsymbol{\Omega}) \,.$$

This is a simple model for so-called *double bracket dissipation* [see Blo+96], which is known to preserve Casimir functions such as

$$C = \mathbf{M}^2 = (I_x \Omega_x)^2 + (I_y \Omega_y)^2 + (I_z \Omega_z)^2 \,.$$

The integrator does not preserve this function exactly, being a general quadratic invariant, although it seems to be preserved in the free case.

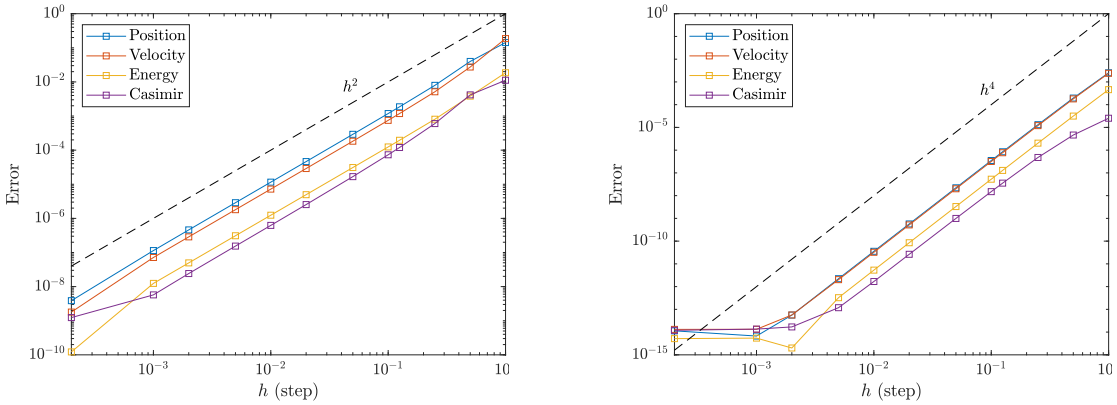


Figure 4.5: Numerical error for separate magnitudes of the model for 2-stage (left) and 3-stage (right) partitioned Lobatto methods.

We chose to discretize the corresponding generalized Lagrangian, $\boldsymbol{\ell}_f$, using Lobatto schemes of 2, 3 stages only, as Lie group integrators are computationally more demanding. The order of an s-stage Lobatto method is $p = 2s - 2$, so the resulting numerical methods are of order 2, 4 respectively. As retraction we have used the standard Cayley map, cay. The parameters used for the numerical simulations shown here are $I = \mathrm{diag}(I_x, I_y, I_z) = (1/2, 2, 1)$ and $\alpha = 1$, for no particular reason. The other choices of parameters that were tested showed essentially the same behaviour. We run each simulation for a total of 1 unit of simulation time with several different choices of step-size h ranging between $1 \cdot 10^{-4}$ and 1 and measure numerical error as the difference between the final value of the magnitude being studied found for a reference simulation and the corresponding one for the value we want to study. In this case our reference is taken as the simulation with the finest step-size. The initial values chosen for the results in figure 4.5 are $(\Omega_x, \Omega_y, \Omega_z) = (1/\sqrt{2}, 0, 1/\sqrt{2})$.

For the resolution of the resulting non-linear system of equations derived for each method, we used MATLAB's `fsolve` with `TolX=1e-12` and `TolX=1e-14` respectively.

Chapter 5

High-order methods for constrained systems

In this chapter we will propose and analyze a new integration scheme for systems of index 2 (see section 2.3.5). After that we will check how this scheme and these results can be applied to the geometric integration of nonholonomic mechanical systems (see section 5.1) on vector spaces, Lie groups and even for optimal control problems involving these systems.

Chronologically, the development was in fact inverted. First, we tackled the problem of numerical integration of nonholonomic mechanical systems, for which no systematic error analysis exists as of yet as it falls outside the scope of the variational error theorem (thm. 3.2.2). In fact, even the existence of an exact discrete Lagrangian in the nonholonomic setting is still an active research topic in the community. This was the initial motivation to study forced systems, fueling the developments of chapter 4. In the end we were not able to advance any further along that route in regard to the nonholonomic problem.

Meanwhile, we proposed a scheme for high order methods for nonholonomic systems inspired by the geometric interpretation of these systems and of variational integrators. As we were not capable of applying our results on forced systems to analyze this new scheme, it was clear that a deeper numerical analysis had to be done. This allowed us to prove the order of the scheme. Once the foundations were laid, we were free to work on extending the scheme to nonholonomic systems on Lie groups and even to the optimal control setting. The corresponding sections are part of a pair of papers, currently under consideration and available as preprints [Sat18; MS18a].

We will first look into the geometric description of constrained mechanical systems in the continuous setting, both in the holonomic and nonholonomic case, and later we will move on to the discrete case.

Before the section on discrete nonholonomic mechanics we offer a brief exposition about the discrete holonomic case, which will hopefully provide an even clearer picture of how and why this method was created.

5.1 Constrained mechanical systems

In this section we will provide a brief overview of the continuous mechanics for constrained systems. We will consider both the holonomic and the nonholonomic case in the augmented setting, as it will be key for our developments for numerical methods in the next sections.

5.1.1 Lagrangian description

Holonomically constrained systems

As we saw in section 2.2.3, every time we consider a variational problem on a manifold it can be considered a constrained problem on its own. Thus, it should come as no surprise that a *holonomically constrained* Lagrangian system (i.e. one where the constraints are imposed directly on the configuration manifold) is not a big departure from what we have studied up until now.

Assume we have a Lagrangian system (Q, L) and a constraint submanifold N embedded in our space Q, with $i_N : N \hookrightarrow Q$. Then (Q, L, N) is a constrained Lagrangian system. Observe that by differentiation this inclusion provides us with a canonical way to embed TN in TQ, that is $Ti_N : TN \hookrightarrow TQ$. Then, if we define the **constrained Lagrangian** $L^N = L \circ Ti_N$, the constrained system can be simply recast as a new free Lagrangian system (N, L^N).

The real departure comes when we insist on viewing the system as living in Q (which will be important for us in the next section when considering nonholonomic mechanics). In this case the submanifold N will be locally defined by the null-set of a function $\Phi : Q \to V$ (i.e. $\Phi^{-1}(0) = N$), where V is an inner product space with $\dim V = m = \operatorname{codim} N$. We will commonly consider $V \equiv \mathbb{R}^m$. As in section 2.2.3 we can tackle the problem by using Lagrange multipliers. The idea is to extend our configuration space Q into a trivial product space $Q \times V$. If $\lambda \in V$, using local coordinates $\lambda = (\lambda^i)$, $i = 1, ..., m$, then we may write the **augmented Lagrangian** $\tilde{L} : TQ \times V \to \mathbb{R}$ as

$$\tilde{L}(q, v, \lambda) = L(q, v) + \langle \lambda, \Phi(q) \rangle \tag{5.1}$$

where here $\langle \cdot, \cdot \rangle$ denotes the inner product in V.

Direct application of Hamilton's principle on $Q \times V$ yields the system of equations:

$$\begin{gathered} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = \left\langle \lambda, \frac{\partial \Phi}{\partial q^i} \right\rangle, \quad \text{for } i = 1, ..., n\,, \\ \Phi(q) = 0\,. \end{gathered}$$

The form of these equations is interesting as it shows that the extra terms due to the constraining of the system appear as forcing terms (cf. section 4.1.1). Therefore, these receive the name of *constraint forces* [Arn89; Whi88; GPS02].

Nonholonomic mechanics

Nonholonomic mechanics is the study of mechanical systems whose evolution is constrained depending on both its current position and velocity. More rigorously, the nonholonomic constraints are specified by a submanifold $N \subset TQ$ (cf. holonomic case $N \subset Q$). In most applications N is a vector subbundle which is completely described by a non-integrable distribution $\mathcal{D}$ and so one identifies $N \equiv \mathcal{D}$, although that need not be the case for us. Thus, let us state the following:

Definition 5.1.1. A **nonholonomic mechanical system** is a triple (L, Q, N) where $L : TQ \to \mathbb{R}$ is a C^k regular Lagrangian, with $k \geq 2$, and $N \subset TQ$ such that $N \neq TX$ for some $X \subset Q$.

In what follows we will assume for simplicity that $\tau_Q(N) = Q$, where $\tau_Q : TQ \to Q$. See more details in [Blo15; Cor02; NF72].

One is commonly given a function $\Phi : TQ \to V \equiv \mathbb{R}^m$, with $m = \operatorname{codim}_{TQ}(N)$ such that its null-set is N. If $i_N : N \to TQ$, then we could define a restricted Lagrangian, $L^N = L \circ i_N$, and *a priori* this latter description would be the most natural for the system but that is not necessarily true [see Gra+09]. In fact, for a nonholonomic Lagrangian system the equations of motion still rely on the complete Lagrangian L. Only a subset, albeit an important one, of these systems admits a complete description in terms of L^N, the constrained variational system or vakonomic systems [see Cor02].

An important space that will appear later is the Chetaev bundle, $S^*(TM^0)$, where $(TM)^0 \subseteq T^*Q$ denotes the annihilator of TM. This is locally spanned by $S^*(\mathrm{d}\Phi)$, which can be understood as a set of separated semibasic 1-forms

$$\frac{\partial \Phi^a}{\partial v^i} \mathrm{d}q^i, \quad \forall a = 1, ..., m.$$

It will always be assumed that Φ is such that $\operatorname{rank} S^*(\mathrm{d}\Phi) = m$ (*admissibility condition*). Additionally, we will assume that L and Φ satisfy that the matrix whose elements are:

$$C^{ab} = g_L^{ij} \frac{\partial \Phi^a}{\partial v^i} \frac{\partial \Phi^b}{\partial v^j},$$

where g_L^{ij} are the elements of the inverse of $(g_L)_{ij}$, is regular (*compatibility condition*) [see LM96].

Once we are given a nonholonomic mechanical system, the next thing to do is to obtain its corresponding equations of motion. Mathematically it is easier to formulate the equations of motion for the (L, Φ) system in an augmented setting through the method of Lagrange multipliers. There exists an intrinsic derivation of the equations in N (restricted setting) which sidesteps the use of these multipliers, but we will use the former. It is well known that the equations of motion of a nonholonomic system are not described using standard constrained variational calculus for L^N [see LM95].

The main departure point of nonholonomic mechanics from its holonomic counterpart is that its evolution equations are non-variational, i.e. they cannot be derived from a purely variational principle like Hamilton's principle. As we will see in a moment, we will need to use *Chetaev's principle* instead, which can be understood as an instance of the Lagrange-D'Alembert principle for a particular kind of constraints (linear or affine) [LM96; Cor02].

Consider the submanifold $\widetilde{C}^2(q_a, q_b, [t_a, t_b])$ of $C^2(q_a, q_b, [t_a, t_b])$, consisting of the curves which are compatible with the constraint:

$$\widetilde{C}^2(q_a, q_b, [t_a, t_b]) = \left\{ \tilde{c} \in C^2(q_a, q_b, [t_a, t_b]) \mid \left(\tilde{c}(t), \dot{\tilde{c}}(t)\right) \in N \right\}.$$

For each $\tilde{c} \in \widetilde{C}^2(q_a, q_b, [t_a, t_b])$ we can consider the vector subspace of $T_{\tilde{c}} C^2(q_a, q_b, [t_a, t_b])$,

$$\begin{aligned} \mathcal{V}^\Phi_{\tilde{c}}(q_a, q_b, [t_a, t_b]) = \Big\{ & X \in T_{\tilde{c}} C^2(q_a, q_b, [t_a, t_b]) \mid \forall \bar{X}(t) \in T_{(\tilde{c}(t), \dot{\tilde{c}}(t))} TQ \\ & \text{s.t. } T\tau_Q\left(\bar{X}\right) = X, S^*\left(\mathrm{d}\Phi\right)\left(\bar{X}\right) = 0 \Big\}. \end{aligned}$$

Given a vector field along a solution $\tilde{c}$, $X = X^i \frac{\partial}{\partial q^i}$, then $X \in \mathcal{V}^\Phi_{\tilde{c}}(q_a, q_b, [t_a, t_b])$ if and only if:

$$X^i \frac{\partial \Phi^a}{\partial \dot{q}^i}\Big|_{\tilde{c}} = 0, \quad \forall a = 1, ..., m. \qquad \text{(variational constraint)}$$

Definition 5.1.2. (Chetaev's principle). A curve $\tilde{c} \in \tilde{C}^2(q_a, q_b, [t_a, t_b])$ is a solution of the nonholonomic Lagrangian system defined by $L : TQ \to \mathbb{R}$ and $\Phi : TQ \to \mathbb{R}^m$ if and only if $\tilde{c}$ satisfies $\mathrm{d}\mathcal{J}(\tilde{c})(X) = 0$, for all $X \in \mathcal{V}^{\Phi}_{\tilde{c}}(q_a, q_b, [t_a, t_b])$.

This means that $\tilde{c}$ is a solution of the nonholonomic problem if and only if:

$$D_{\mathrm{EL}} L \left(\hat{\tilde{c}}^{(2)} \right) (X) = \left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} \right) X^i = 0,$$

for all X^i satisfying the variational constraint, i.e. $D_{\mathrm{EL}} L(\tilde{c})$ is in the Chetaev bundle. This implies that the equations of motion can be written as:

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = \left\langle \lambda, \frac{\partial \Phi}{\partial \dot{q}^i} \right\rangle, \quad \text{for } i = 1, ..., n; \tag{5.2}$$

where $\lambda_1, ..., \lambda_m$ are Lagrange multipliers. These multipliers are determined by ensuring that the curve belongs to $\widetilde{C}^2(q_a, q_b, [t_a, t_b])$, i.e. imposing the constraint equations:

$$\Phi(q, \dot{q}) = 0. \tag{5.3}$$

To ensure that the resulting system of equations for the multipliers has a unique solution, it is necessary to invoke the *compatibility condition* ((C^{ab}) is a regular matrix or see next section).

Note that, as in the standard case, due to the regularity of the Lagrangian we can write the Euler-Lagrange equations as a second order equation

$$\ddot{q}^i(t) = F^i(q, \dot{q}, \lambda)\,.$$

Then, the equation for the multipliers can be obtained by differentiating the constraint and inserting this last equation, that is,

$$\frac{\partial \Phi}{\partial q^i} \dot{q}^i + \frac{\partial \Phi}{\partial \dot{q}^i} F^i(q, \dot{q}, \lambda) = 0\,.$$

Under the conditions stated it is possible to solve for $\lambda = \lambda(q, \dot{q})$.

When the constraints are linear, which is by far the most common case, it is possible to write them as $\Phi^\alpha(q, v) = \varphi^\alpha_i(q) v^i$, with $\varphi^\alpha \in \Omega^1(Q)$ for $\alpha = 1, ..., m$. In this case the system simplifies to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} &= \lambda_\alpha \varphi^\alpha_i(q)\,, \\ \varphi^\alpha_i(q) \dot{q}^i &= 0\,. \end{aligned}$$

Note that the resulting equations from the application of the Chetaev principle, eq.(5.2), do not coincide with those obtained in the variational nonholonomic case (cf. eq.(2.10)). Numerous physical experiments have been carried out that show that the latter have nothing to do with the behavior of a true nonholonomic system [LM95]. Nevertheless, those equations are interesting in their own right, as they are closely related to optimal control problems [Blo15] and subriemannian geometry [Mon02].

Geometric description

Geometrically the equations of motion derived from Chetaev's principle can be reformulated as:

$$\imath_X \omega_L - \mathrm{d}E_L \in F^0_{\mathrm{nh}},$$

where $X \in TN$ and $F^0_{\mathrm{nh}} = S^*((TN)^0)$ is the Chetaev bundle. Define also the space $F^\perp_{\mathrm{nh}}$ by $\flat_L \left(F^\perp_{\mathrm{nh}}\right) = F^0_{\mathrm{nh}}$ where $\flat_L : T(TQ) \to T^*(TQ)$ and $\sharp_L : T^*(TQ) \to T(TQ)$ are the musical endomorphisms defined by ω_L, that is, $\flat_L(X) = i_X\omega_L$ and $\sharp_L = (\flat_L)^{-1}$. The regularity assumption about a nonholonomic system stated above can be recast as:

- $\operatorname{codim} N = \operatorname{rank} F^0_{\mathrm{nh}}$ (*admissibility condition*),
- $TN \cap F^\perp_{\mathrm{nh}} = 0$ (*compatibility condition*).

A solution X will be of the form $X = \xi_L + \lambda_b \zeta^b$, where ξ_L is the Hamiltonian vector field of the unconstrained problem and $\zeta^a = \sharp_L(S^*(\mathrm{d}\Phi^a))$. To determine the Lagrange multipliers we need to use the tangency condition $X(\Phi) = 0$, where we get:

$$X(\Phi^a) = \xi_L(\Phi^a) + \lambda_b \zeta^b(\Phi^a) = 0 \tag{5.4}$$

where $\zeta^b(\Phi^a) = C^{ba}$. In [CR93; LM96; LMM97] it is shown that the regularity of this matrix implies the geometric compatibility condition just stated.

5.1.2 Hamiltonian description

Holonomically constrained system

We will not be discussing the intrinsic setting for the holonomic case, where we would work in T^*N. We will instead comment only on the augmented setting.

Consider a Hamiltonian $H : T^*Q \to \mathbb{R}$ and a constraint submanifold $N \subset Q$ defined by the null-set of $\Phi : Q \to \mathbb{R}^m$. Let $T^*(Q \times \mathbb{R}^m) \equiv T^*Q \times \mathbb{R}^{2m}$ be the augmented phase space with projection $\mu : T^*(Q \times \mathbb{R}^m) \to T^*Q$. We can then define an augmented Hamiltonian $\widetilde{H} : T^*(Q \times \mathbb{R}^m) \to \mathbb{R}$

$$\widetilde{H}(q, \lambda, p, \pi) = H(q, p) - \langle \lambda, \Phi(q) \rangle$$

where π denotes the conjugate variable of λ which does not appear. (The sign was chosen so that the multipliers appear with the same sign as in the Lagrangian side.)

Let $\tilde{\omega}_Q$ denote the pull-back to $T^*(Q \times \mathbb{R}^m)$ of the canonical symplectic form on T^*Q, i.e. $\tilde{\omega}_Q = \mu^*\omega_Q$. Note that this form is degenerate. With it, the Hamilton equations of motion can be written as

$$\imath_{X_{\widetilde{H}}} \tilde{\omega}_Q = \mathrm{d}\widetilde{H},$$

which in coordinates take the form

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i}\,, \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i} + \left\langle \lambda, \frac{\partial \Phi}{\partial q^i}(q) \right\rangle\,, \\ 0 &= \Phi(q)\,. \end{aligned}$$

Nonholonomic Hamiltonian system

The nonholonomic problem from the Hamiltonian point of view can be described by a function $H : T^*Q \to \mathbb{R}$ and a constraint submanifold $M \subset T^*Q$ with $\mathrm{codim}_{T^*Q} M = m$ [Mar98]. This manifold can be locally described by a function $\Psi : T^*Q \to \mathbb{R}^m$.

In order to derive the Hamiltonian description we will rely on the Lagrangian description of the Chetaev bundle and pull it back using the Legendre transform $\mathbb{F}H$ induced by our Hamiltonian. This forces us to assume that H must be regular. The matrix in eq.(3.5) allows us to define a definite quadratic form $g_H : T^*Q \times T^*Q \to \mathbb{R}$ with corresponding isomorphisms $\sharp_H : T^*Q \to TQ$ and $\flat_H : TQ \to T^*Q$. Thus, the Hamiltonian Chetaev bundle $(F^0_{\mathrm{nh}})^*$ can be locally described by $\flat_H \left(T\tau_Q \left(\sharp_\omega \mathrm{d}\Psi\right)\right)$, where $\sharp_\omega : T^*(T^*Q) \to T(T^*Q)$ is the musical isomorphism induced by the canonical structure and $T\tau_Q : T(T^*Q) \to TQ$.

Similar to the Lagrangian case, the resulting equations of motion are:

$$\imath_X \omega_Q - \mathrm{d}H \in \left(F^0_{\mathrm{nh}}\right)^* .$$

Using the notation $(g_H)_{ij}$ for the elements of the inverse of $g_H^{ij} = \frac{\partial^2 H}{\partial p_i \partial p_j}$, we can write these equations in local coordinates as:

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i}, \qquad \forall i = 1, ..., n \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i} + \left\langle \lambda, (g_H)_{ij} \frac{\partial \Psi}{\partial p_j} \right\rangle , \end{aligned}$$

together with the constraint equations

$$\Psi(q, p) = 0.$$

In the linear case, this system can be simply written as

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p_i}, \qquad \forall i = 1, ..., n \\ \dot{p}_i &= -\frac{\partial H}{\partial q^i} + \lambda_\alpha \varphi_i^\alpha(q), \\ 0 &= \varphi_i^\alpha(q) \frac{\partial H}{\partial p_i}, \quad \forall \alpha = 1, ..., m. \end{aligned}$$

5.2 Numerical analysis of partitioned systems of index 2

Let N, M be smooth manifolds such that $M \subseteq N$. Assume that $\dim N = n$ and $\mathrm{codim} M = m$ and let M be defined as the null-set of $\phi : N \to \mathbb{R}^m$. A generic explicit differential equation on M can be recast into a semi-explicit index 2 differential algebraic equation (DAE) on N taking the form:

$$\left\{ \begin{array}{ll} \dot{y} & = f(y, z) \\ 0 & = \phi(y) \end{array} \right. \tag{5.5}$$

where $y \in N$ and $z \in V$, with V a vector space such that $\dim V = m$. Studies on the numerical solution of initial value problems (IVP) for such general systems on vector

spaces can be found in the bibliography that serves as foundation for this chapter, such as [HLR89] or [Jay93].

We are interested in a subset of such problems, which will be referred to as *partitioned*, where $y = (q, p)$, $\dim Q = \dim P = n$ (thus, in this case $\dim N = 2n$), and $\lambda \in \mathbb{R}^m$.

$$\begin{cases} \dot{q} &= f(q,p) \\ \dot{p} &= g(q,p,\lambda) \\ 0 &= \phi(q,p)\,. \end{cases} \tag{5.6}$$

Such is the case of the equations of motion of nonholonomic mechanical systems, which motivates our study. Remember that nonholonomic equations are in Hamiltonian form (see section 5.1.2)

$$\begin{cases} \dot{q}^i = \dfrac{\partial H}{\partial p_i}, & \forall i = 1, ..., n \\ \dot{p}_i = -\dfrac{\partial H}{\partial q^i} + \lambda_\alpha \left(g_H\right)_{ij} \dfrac{\partial \Psi^\alpha}{\partial p_j}, & \\ 0 = \Psi^\alpha(q,p), & \forall \alpha = 1, ..., m \end{cases} \tag{5.7}$$

for a Hamiltonian function $H(q,p)$ and nonholonomic constraints $\Psi^\alpha(q,p) = 0$. An IVP for this partitioned DAE is defined by an initial condition $(q_0, p_0, \lambda_0) \in N|_M \times \mathbb{R}^m$.

For the remainder of the chapter we will assume that f, g and ϕ are sufficiently differentiable and that the matrix

$$\left(D_2\phi \cdot D_3 g\right)(q,p,\lambda) = \left(\frac{\partial \phi^\alpha}{\partial p_j}(q,p)\frac{\partial g_j}{\partial \lambda_\beta}(q,p,\lambda)\right)$$

remains invertible in a neighborhood of the exact solution. Here D_i means derivative with respect to the i-th argument, and i acts as a multi-index.

5.2.1 Lobatto-type methods

Assuming N is a vector space, a numerical solution of an IVP for (5.5) can be found using an s-stage Runge-Kutta method with coefficients (a_{ij}, b_j) (see section 2.3.1). Writing the corresponding equations is a relatively trivial matter, taking the form:

$$y_1 = y_0 + h\sum_{j=1}^{s} b_j k_j, \qquad z_1 = z_0 + h\sum_{j=1}^{s} b_j l_j \tag{5.8a}$$

$$Y_0^i = y_0 + h\sum_{j=1}^{s} a_{ij} k_j, \quad Z_0^i = z_0 + h\sum_{j=1}^{s} a_{ij} l_j \tag{5.8b}$$

$$k_i = f(Y_0^i, Z_0^i), \qquad 0 = g(Y_0^i). \tag{5.8c}$$

Note that these l_j are not given explicitly and must instead be solved for with the help from the constraint equations. In fact, provided the RK coefficients satisfy certain conditions, we may eliminate the equations for the z and Z variables completely.

Now, a numerical solution of an IVP for eqs.(5.6) can also be found using an s-stage *partitioned* Runge-Kutta method but already the correct application of such a scheme is

non-trivial. One could naively write:

$$q_1 = q_0 + h\sum_{j=1}^{s} b_j V_0^j, \quad p_1 = p_0 + h\sum_{j=1}^{s} \hat{b}_j W_0^j, \quad \lambda_1 = \lambda_0 + h\sum_{j=1}^{s} \check{b}_j U_0^j, \tag{5.9a}$$

$$Q_0^i = q_0 + h\sum_{j=1}^{s} a_{ij} V_0^j, \quad P_0^i = p_0 + h\sum_{j=1}^{s} \hat{a}_{ij} W_0^j, \quad \Lambda_0^i = \lambda_0 + h\sum_{j=1}^{s} \check{a}_{ij} U_0^j, \tag{5.9b}$$

$$V_0^i = f(Q_0^i, P_0^i), \qquad W_0^i = g(Q_0^i, P_0^i, \Lambda_0^i), \qquad 0 = \phi(Q_0^i, P_0^i). \tag{5.9c}$$

Again, U_0^j are not given explicitly and, as above, in some cases, it may also be possible to eliminate the equations for λ and Λ. Unfortunately, such a system of equations may have certain issues, both from a solvability point of view and from a numerical convergence point of view. This is especially true for the particular case of partitioned Runge-Kutta methods that we will consider.

In [Jay93] the author considers Runge-Kutta methods satisfying the hypotheses:

H1 $a_{1j} = 0$ for $j = 1, ..., s$;

H2 the submatrix $\tilde{A} := (a_{ij})_{i,j\geq 2}$ is invertible;

H3 $a_{sj} = b_j$ for $j = 1, ..., s$ (the method is *stiffly accurate*).

H1 implies that $c_1 = \sum_{j=1}^{s} a_{1j} = 0$ and for eqs.(5.8) $Y_1 = y_0$, $\Lambda_1 = \lambda_0$. H3 implies that $y_1 = Y_s$, $\lambda_1 = \Lambda_s$. Furthermore, if the method is *consistent*, i.e. $\sum_j b_j = 1$, then H3 implies $c_s = 1$. For eqs.(5.9), if $(\check{a}_{ij}, \check{b}_j)$ also satisfies the hypotheses, then $Q_1 = q_0$, $\Lambda_1 = \lambda_0$, $Q_s = q_1$ and $\Lambda_s = \lambda_1$. The most salient example of these methods is the **Lobatto IIIA**, which is a continuous collocation method.

The **Lobatto IIIB** is a family of discontinuous collocation methods which are symplectically conjugated to the IIIA methods. Two Runge-Kutta methods, (a_{ij}, b_j) and $(\hat{a}_{ij}, \hat{b}_j)$, satisfying the *compatibility condition* $\sum_{j=1}^{s} \hat{a}_{ij} = \hat{c}_i = c_i = \sum_{j=1}^{s} a_{ij}$, are symplectically conjugated if they satisfy:

$$b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j \quad \text{for } i, j = 1, ..., s\,, \tag{5.10}$$

$$b_j = \hat{b}_j \quad \text{for } j = 1, ..., s\,. \tag{5.11}$$

Together they form the **Lobatto IIIA-IIIB** family of **symplectic partitioned Runge-Kutta** methods, which is precisely the one we want to study [see also NW81; HLW10].

Note that Lobatto IIIB methods do not satisfy any of the hypotheses aforementioned. In fact, any symplectic conjugate method to a method satisfying those hypotheses must necessarily be such that:

H1' $\hat{a}_{is} = 0$ for $i = 1, ..., s$;

H2' $\hat{a}_{i1} = \hat{b}_1$ for $i = 1, ..., s$.

Obviously, the submatrix $\tilde{\hat{A}} := (\hat{a}_{ij})_{i,j\geq 2}$ is never invertible because of H1', and this is the culprit of the solvability issues of (5.9).

For such methods, we propose the following equations for the numerical solution of the partitioned IVP:

$$q_1 = q_0 + h\sum_{j=1}^{s} b_j V_0^j, \qquad p_1 = p_0 + h\sum_{j=1}^{s} \hat{b}_j W_0^j, \tag{5.12a}$$

$$Q_0^i = q_0 + h\sum_{j=1}^{s} a_{ij} V_0^j, \qquad P_0^i = p_0 + h\sum_{j=1}^{s} \hat{a}_{ij} W_0^j, \tag{5.12b}$$

$$p_0^i = p_0 + h\sum_{j=1}^{s} a_{ij} W_0^j, \qquad 0 = \phi(Q_0^i, p_0^i), \tag{5.12c}$$

$$V_0^i = f(Q_0^i, P_0^i), \qquad W_0^i = g(Q_0^i, P_0^i, \Lambda_0^i), \tag{5.12d}$$

together with $\Lambda_0^1 = \lambda_0$ and $\Lambda_0^s = \lambda_1$. It should be noted that, although similar, these methods do not generally coincide with the SPARK methods proposed by L. O. Jay in [Jay09]. [See Mur97, for a similar approach initially unknown by the author.]

5.2.2 Existence, uniqueness and influence of perturbations

Theorem 5.2.1. *Let $U \subset N \times \mathbb{R}^m$ be a fixed neighborhood of $(q_0, p_0, \lambda_0) = (q_0(h), p_0(h), \lambda_0(h))$, a set of h-dependent starting values, and assume:*

$$\begin{aligned}
&\phi(q_0, p_0) = 0\\
&(D_1\phi \cdot f)(q_0, p_0) + (D_2\phi \cdot g)(q_0, p_0, \lambda_0) = \mathcal{O}(h)\\
&(D_2\phi \cdot D_3 g)(q, p, \lambda) \text{ invertible in } U.
\end{aligned}$$

Assume also that the Runge-Kutta coefficients A verify the hypotheses H1 and H2, and that $\hat{A}$ is compatible with the first and satisfies H1'. Then, for $h \leq h_0$, there exists a locally unique solution to:

$$Q_0^i = q_0 + h\sum_{j=1}^{s} a_{ij} f(Q_0^j, P_0^j), \tag{5.13a}$$

$$p_0^i = p_0 + h\sum_{j=1}^{s} a_{ij} g(Q_0^j, P_0^j, \Lambda_j), \tag{5.13b}$$

$$P_0^i = p_0 + h\sum_{j=1}^{s} \hat{a}_{ij} g(Q_0^j, P_0^j, \Lambda_j), \tag{5.13c}$$

$$0 = \phi(Q_0^i, p_0^i), \tag{5.13d}$$

with $\Lambda_1 = \lambda_0$, satisfying:

$$\begin{aligned}
Q_0^i - q_0 &= \mathcal{O}(h)\,,\\
p_0^i - p_0 &= \mathcal{O}(h)\,,\\
P_0^i - p_0 &= \mathcal{O}(h)\,,\\
\Lambda_0^i - \lambda_0 &= \mathcal{O}(h)\,.
\end{aligned}$$

Proof. The proof of existence differs little from what is already offered in [HLR89] (for invertible A matrices) or [Jay93] (for A satisfying the hypotheses H1 and H2). The idea is to consider a homotopic deformation of the equations which leads to a system of differential equations where the existence of a solution for the corresponding IVP implies the existence of a solution to the original system.

The proposed homotopy is:

$$
\begin{aligned}
Q_0^i &= q_0 + h\sum_{j=1}^{s} a_{ij}\left[f(Q_0^j, P_0^j) + (\tau-1)f(q_0,p_0)\right] \\
p_0^i &= p_0 + h\sum_{j=1}^{s} a_{ij}\left[g(Q_0^j, P_0^j, \Lambda_0^j) + (\tau-1)g(q_0,p_0,\lambda_0)\right] \\
P_0^i &= p_0 + h\sum_{j=1}^{s} \hat{a}_{ij}\left[g(Q_0^j, P_0^j, \Lambda_0^j) + (\tau-1)g(q_0,p_0,\lambda_0)\right] \\
0 &= \phi(Q_0^i, p_0^i) + (\tau-1)\phi(q_0,p_0)
\end{aligned}
$$

where now Q_0^i, p_0^i, P_0^i and Λ_0^i, with $i = 1, ..., s$, are assumed to implicitly depend on τ.

The main differences in the proof lie in the complementary relation between the equations for p_0^i and P_0^i. One needs to consider the differential system obtained by derivation with respect to the homotopy parameter τ. The resulting system takes the form:

$$\dot{Q}_0^i = h\sum_{j=1}^{s} a_{ij}\left[D_1 f(Q_0^j, P_0^j)\dot{Q}_0^j + D_2 f(Q_0^j, P_0^j)\dot{P}_0^j + f(q_0,p_0)\right] \tag{5.14a}$$

$$\begin{aligned}\dot{p}_0^i = h\sum_{j=1}^{s} a_{ij}\Big[&D_1 g(Q_0^j, P_0^j, \Lambda_0^j)\dot{Q}_0^j + D_2 g(Q_0^j, P_0^j, \Lambda_0^j)\dot{P}_0^j \\ &+ D_3 g(Q_0^j, P_0^j, \Lambda_0^j)\dot{\Lambda}_0^j + g(q_0,p_0,\lambda_0)\Big]\end{aligned} \tag{5.14b}$$

$$\begin{aligned}\dot{P}_0^i = h\sum_{j=1}^{s} \hat{a}_{ij}\Big[&D_1 g(Q_0^j, P_0^j, \Lambda_0^j)\dot{Q}_0^j + D_2 g(Q_0^j, P_0^j, \Lambda_j)\dot{P}_0^j \\ &+ D_3 g(Q_0^j, P_0^j, \Lambda_j)\dot{\Lambda}_0^j + g(q_0,p_0,\lambda_0)\Big]\end{aligned} \tag{5.14c}$$

$$0 = D_1\phi(Q_0^i, p_0^i)\dot{Q}_0^i + D_2\phi(Q_0^i, p_0^i)\dot{p}_0^i + \phi(q_0,p_0)\,. \tag{5.14d}$$

Note that $\dot{p}_0^i$ depends on $\dot{Q}_0^j, \dot{P}_0^j, \dot{\Lambda}_0^j$, but not on $\dot{p}_0^j$. In fact, $\dot{p}_0^i$ only appears in eq.(5.14d), where it prevents the entrance of $\hat{a}$ terms. Thus, the differential system that must be solved can be reduced to the $\dot{P}_0^j$, $\forall j = 1, ..., s$ and $\dot{Q}_0^j, \dot{\Lambda}_0^j$, $\forall j = 2, ..., s$ variables. The rest of the proof follows closely what the other authors do.

A remark worth mentioning is that the key of the remainder of the proof is the use of the invertibility of $D_2\phi(\tilde{A}\otimes I)D_3 g$, which is a term arising from eq.(5.14d). As stated in the former section, if the system were described by eq. (5.9) we would instead have $D_2\phi(\hat{\tilde{A}}\otimes I)D_3 g$, which is not invertible by H1', rendering the system unsolvable.

The proof of uniqueness remains essentially the same. □

Theorem 5.2.2. *Under the assumptions of theorem 5.2.1, let Q_0^i, p_0^i, P_0^i, Λ_0^i be the solution of the system in said theorem. Now consider the perturbed values $\hat{Q}_0^i$, $\hat{p}_0^i$, $\hat{P}_0^i$, $\hat{\Lambda}_0^i$*

satisfying:

$$\hat{Q}_0^i = \hat{q}_0 + h\sum_{j=1}^{s} a_{ij} f(\hat{Q}_0^j, \hat{P}_0^j) + h\delta_{Q,i} \tag{5.15a}$$

$$\hat{p}_0^i = \hat{p}_0 + h\sum_{j=1}^{s} a_{ij} g(\hat{Q}_0^j, \hat{P}_0^j, \hat{\Lambda}_0^j) + h\delta_{p,i} \tag{5.15b}$$

$$\hat{P}_0^i = \hat{p}_0 + h\sum_{j=1}^{s} \hat{a}_{ij} g(\hat{Q}_0^j, \hat{P}_0^j, \hat{\Lambda}_0^j) + h\delta_{P,i} \tag{5.15c}$$

$$0 = \phi(\hat{Q}_0^i, \hat{p}_0^i) + \theta_i \tag{5.15d}$$

with $\hat{\Lambda}_1 = \hat{\lambda}_0$*, and where* $\delta_{Q,i}$*,* $\delta_{p,i}$*,* $\delta_{P,i}$ *and* θ_i *are perturbation terms. Additionally, assume that:*

$$\begin{aligned} \hat{q}_0 - q_0 &= \mathcal{O}(h)\,, \\ \hat{p}_0 - p_0 &= \mathcal{O}(h)\,, \\ \delta_{Q,i}, \delta_{p,i}, \delta_{P,i} &= \mathcal{O}(h)\,, \\ \theta_i &= \mathcal{O}(h^2)\,. \end{aligned} \tag{5.16}$$

Then, using the notation $\Delta X := \hat{X} - X$ *and* $\|X\| := \max_i \|X_i\|$*, for small* h *we have:*

$$\begin{aligned} \left\|\Delta Q_0^i\right\| &\le C\left(\|\Delta q_0\| + h\|\Delta p_0\| + h^2\|\Delta\lambda_0\| + h\|\delta_Q\| + h^2\|\delta_p\| + h^2\|\delta_P\| + h\|\theta\|\right) \\ \left\|\Delta p_0^i\right\| &\le C\left(\|\Delta q_0\| + \|\Delta p_0\| + h^2\|\Delta\lambda_0\| + h^2\|\delta_Q\| + h\|\delta_p\| + h^2\|\delta_P\| + \|\theta\|\right) \\ \left\|\Delta P_0^i\right\| &\le C\left(\|\Delta q_0\| + \|\Delta p_0\| + h\|\Delta\lambda_0\| + h^2\|\delta_Q\| + h\|\delta_p\| + h\|\delta_P\| + \|\theta\|\right) \\ \left\|\Delta\Lambda_0^i\right\| &\le \frac{C}{h}\left(h\|\Delta q_0\| + h\|\Delta p_0\| + h\|\Delta\lambda_0\| + h\|\delta_Q\| + h\|\delta_p\| + \|\theta\|\right)\,. \end{aligned}$$

Proof. To tackle this problem we first subtract eq.(5.13) from eq.(5.15) and linearize, obtaining:

$$\begin{aligned} \Delta Q_0^i &= \Delta q_0 + h\sum_{j=1}^{s} a_{ij}\left[D_1 f(Q_0^j, P_0^j)\Delta Q_0^j + D_2 f(Q_0^j, P_0^j)\Delta P_0^j\right] + h\delta_{Q,i} \\ &\quad + \mathcal{O}\left(h\|\Delta Q_0\|^2 + h\|\Delta P_0\|^2 + h\|\Delta Q_0\|\|\Delta P_0\|\right) \\ \Delta p_0^i &= \Delta p_0 + h\sum_{j=1}^{s} a_{ij}\left[D_1 g(Q_0^j, P_0^j, \Lambda_0^j)\Delta Q_0^j + D_2 g(Q_0^j, P_0^j, \Lambda_0^j)\Delta P_0^j\right. \\ &\quad \left. + D_3 g(Q_0^j, P_0^j, \Lambda_0^j)\Delta\Lambda_0^j\right] + h\delta_{p,i} + \mathcal{O}\left(h\|\Delta Q_0\|^2 + h\|\Delta P_0\|^2\right. \\ &\quad \left. + h\|\Delta Q\|\|\Delta P_0\| + h\|\Delta Q_0\|\|\Delta\Lambda_0\| + h\|\Delta P_0\|\|\Delta\Lambda_0\|\right) \\ \Delta P_0^i &= \Delta p_0 + h\sum_{j=1}^{s} \hat{a}_{ij}\left[D_1 g(Q_0^j, P_0^j, \Lambda_0^j)\Delta Q_0^j + D_2 g(Q_0^j, P_0^j, \Lambda_0^j)\Delta P_0^j\right. \\ &\quad \left. + D_3 g(Q_0^j, P_0^j, \Lambda_0^j)\Delta\Lambda_0^j\right] + h\delta_{P,i} + \mathcal{O}\left(h\|\Delta Q_0\|^2 + h\|\Delta P_0\|^2\right. \\ &\quad \left. + h\|\Delta Q_0\|\|\Delta P_0\| + h\|\Delta Q_0\|\|\Delta\Lambda_0\| + h\|\Delta P_0\|\|\Delta\Lambda_0\|\right) \\ 0 &= D_1\phi(Q_0^i, p_0^i)\Delta Q_0^i + D_2\phi(Q_0^i, p_0^i)\Delta p_0^i + \theta_i \\ &\quad + \mathcal{O}\left(\|\Delta Q_0\|^2 + \|\Delta p_0\|^2 + \|\Delta Q_0\|\|\Delta p_0\|\right)\,. \end{aligned}$$

We will write this system of equations as separate matrix subsystems:

$$\begin{bmatrix} \Delta Q_0^1 \\ \Delta \tilde{Q} \\ \Delta P_0^1 \\ \Delta \tilde{P} \end{bmatrix} = \begin{bmatrix} \Delta q_0 \\ I_{s-1}\otimes \Delta q_0 \\ \Delta p_0 \\ I_{s-1}\otimes \Delta p_0 \end{bmatrix} + h \begin{bmatrix} \delta_{Q,1} \\ \tilde{\delta}_Q \\ \delta_{P,1} \\ \tilde{\delta}_P \end{bmatrix} + h \begin{bmatrix} a_{11}\otimes I_n & \tilde{A}^1\otimes I_n & 0 & 0 \\ \tilde{A}_1\otimes I_n & \tilde{A}\otimes I_n & 0 & 0 \\ 0 & 0 & \hat{a}_{11}\otimes I_n & \hat{\tilde{A}}^1\otimes I_n \\ 0 & 0 & \hat{\tilde{A}}_1\otimes I_n & \hat{\tilde{A}}\otimes I_n \end{bmatrix}$$
$$\times \left(\begin{bmatrix} D_1 f_1 & 0 & D_2 f_1 & 0 \\ 0 & D_1\tilde{f} & 0 & D_2\tilde{f} \\ D_1 g_1 & 0 & D_2 g_1 & 0 \\ 0 & D_1\tilde{g} & 0 & D_2\tilde{g} \end{bmatrix} \begin{bmatrix} \Delta Q_0^1 \\ \Delta \tilde{Q}_0 \\ \Delta P_0^1 \\ \Delta \tilde{P}_0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ D_3 g_1 & 0 \\ 0 & D_3\tilde{g} \end{bmatrix} \begin{bmatrix} \Delta \Lambda_0^1 \\ \Delta \tilde{\Lambda}_0 \end{bmatrix} \right)$$

$$\begin{bmatrix} \Delta Q_0^1 \\ \Delta \tilde{Q}_0 \\ \Delta p_0^1 \\ \Delta \tilde{p}_0 \end{bmatrix} = \begin{bmatrix} \Delta q_0 \\ I_{s-1}\otimes \Delta q_0 \\ \Delta p_0 \\ I_{s-1}\otimes \Delta p_0 \end{bmatrix} + h \begin{bmatrix} \delta_{Q,1} \\ \tilde{\delta}_Q \\ \delta_{p,1} \\ \tilde{\delta}_p \end{bmatrix} + h \begin{bmatrix} a_{11}\otimes I_n & \tilde{A}^1\otimes I_n & 0 & 0 \\ \tilde{A}_1\otimes I_n & \tilde{A}\otimes I_n & 0 & 0 \\ 0 & 0 & a_{11}\otimes I_n & \tilde{A}^1\otimes I_n \\ 0 & 0 & \tilde{A}_1\otimes I_n & \tilde{A}\otimes I_n \end{bmatrix}$$
$$\times \left(\begin{bmatrix} D_1 f_1 & 0 & D_2 f_1 & 0 \\ 0 & D_1\tilde{f} & 0 & D_2\tilde{f} \\ D_1 g_1 & 0 & D_2 g_1 & 0 \\ 0 & D_1\tilde{g} & 0 & D_2\tilde{g} \end{bmatrix} \begin{bmatrix} \Delta Q_0^1 \\ \Delta \tilde{Q}_0 \\ \Delta P_0^1 \\ \Delta \tilde{P}_0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ D_3 g_1 & 0 \\ 0 & D_3\tilde{g} \end{bmatrix} \begin{bmatrix} \Delta \Lambda_0^1 \\ \Delta \tilde{\Lambda}_0 \end{bmatrix} \right)$$

$$\begin{bmatrix} D_1\phi_1 & 0 & D_2\phi_1 & 0 \\ 0 & D_1\tilde{\phi} & 0 & D_2\tilde{\phi} \end{bmatrix} \begin{bmatrix} \Delta Q_0^1 \\ \Delta \tilde{Q}_0 \\ \Delta p_0^1 \\ \Delta \tilde{p}_0 \end{bmatrix} + \begin{bmatrix} \theta_1 \\ \tilde{\theta} \end{bmatrix} = 0$$

where $\tilde{A}_1 = (a_{i1})$, with $i = 2, ..., s$, and $\tilde{A}^1 = (a_{1j})$, with $j = 2, ..., s$, and similarly with the $\hat{a}$ coefficients.

Let us rewrite this in shorthand notation as:

$$\Delta Y = \Delta\eta + h\delta_Y + h\begin{pmatrix} A & \\ \hat{A} & \end{pmatrix}(D_y F \Delta Y + D_\lambda F \Delta\Lambda_0) \tag{5.17a}$$
$$\Delta y = \Delta\eta + h\delta_y + h\begin{pmatrix} A & \\ A & \end{pmatrix}(D_y F \Delta Y + D_\lambda F \Delta\Lambda_0) \tag{5.17b}$$
$$0 = D_y\phi\Delta y + \theta\,. \tag{5.17c}$$

Using hypothesis H1 we find that:

$$\begin{aligned} \Delta Q_0^1 &= \Delta q_0 + h\delta_{Q,1} \\ \Delta p_0^1 &= \Delta p_0 + h\delta_{p,1} \\ D_1\phi(q_0,p_0)\Delta q_0 + D_2\phi(q_0,p_0)\Delta p_0 &= \mathcal{O}\left(h\|\delta_{Q,1}\| + h\|\delta_{p,1}\| + \|\theta_1\|\right. \\ &\quad \left. + \|\Delta q_0\|^2 + \|\Delta p_0\|^2 + \|\Delta q_0\|\|\Delta p_0\|\right)\,. \end{aligned}$$

Most of the proof will follow the lines of the one of [Jay93]. We will first insert eq.(5.17b) in the constraint eq.(5.17c)

$$D_y\phi\left[\Delta\eta + h\delta_y + h\begin{pmatrix} A & \\ A & \end{pmatrix}(D_y F\Delta Y + D_\lambda F\Delta\Lambda_0)\right] + \theta = 0\,.$$

Our mission will be to solve for $\Delta\Lambda_0$, but due to the singularity of A it will not be possible to solve for the entire vector. Instead, abusing our notation a bit, we will separate the term as $D_\lambda F\Delta\Lambda = D_\lambda F_1\Delta\Lambda_0^1 + D_\lambda\tilde{F}\Delta\tilde{\Lambda}_0$, which leads to:

$$\begin{aligned} -hD_y\phi\begin{pmatrix} A & \\ A & \end{pmatrix}D_\lambda\tilde{F}\Delta\tilde{\Lambda}_0 =& D_y\phi\left[\Delta\eta + h\delta_y + h\begin{pmatrix} A & \\ A & \end{pmatrix}\left(D_y F\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right)\right] \\ &+ \theta\,. \end{aligned}$$

Using H1 and taking into account all the zeros that appear in the rest of the elements, the left-hand side can be reduced to $-hD_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right)D_3\tilde{g}\Delta\tilde{\Lambda}_0$. Solving for $h\Delta\tilde{\Lambda}_0$ we get

in matrix notation:

$$
\begin{aligned}
&h\Delta\tilde{\Lambda}_0 \\
&= -\left[\tilde{0}_1\ \left(D_2\tilde{\phi}\big(\tilde{A}\otimes I_n\big)D_3\tilde{g}\right)^{-1}\right]\left\{\begin{bmatrix}\theta_1\\ \tilde{\theta}\end{bmatrix}+\begin{bmatrix}D_1\phi_1 & 0 & D_2\phi_1 & 0\\ 0 & D_1\tilde{\phi} & 0 & D_2\tilde{\phi}\end{bmatrix}\left[\begin{bmatrix}\Delta q_0\\ I_{s-1}\otimes\Delta q_0\\ \Delta p_0\\ I_{s-1}\otimes\Delta p_0\end{bmatrix}+h\begin{bmatrix}\delta_{Q,1}\\ \tilde{\delta}_Q\\ \delta_{p,1}\\ \tilde{\delta}_p\end{bmatrix}\right.\right. \\
&\quad\left.\left.+\ h\begin{bmatrix}a_{11}\otimes I_n & \tilde{A}^1\otimes I_n & 0 & 0\\ \tilde{A}_1\otimes I_n & \tilde{A}\otimes I_n & 0 & 0\\ 0 & 0 & a_{11}\otimes I_n & \tilde{A}^1\otimes I_n\\ 0 & 0 & \tilde{A}_1\otimes I_n & \tilde{A}\otimes I_n\end{bmatrix}\left(\begin{bmatrix}D_1f_1 & 0 & D_2f_1 & 0\\ 0 & D_1\tilde{f} & 0 & D_2\tilde{f}\\ D_1g_1 & 0 & D_2g_1 & 0\\ 0 & D_1\tilde{g} & 0 & D_2\tilde{g}\end{bmatrix}\begin{bmatrix}\Delta Q_0^1\\ \Delta\tilde{Q}_0\\ \Delta P_0^1\\ \Delta\tilde{P}_0\end{bmatrix}+\begin{bmatrix}0\\ 0\\ D_3g_1\\ 0\end{bmatrix}\Delta\Lambda_0^1\right)\right]\right\}.
\end{aligned}
$$

Let us also introduce the notation

$$
(D_2\phi AD_3g)^- = \begin{bmatrix}0 & \tilde{0}^1\\ \tilde{0}_1 & \left(D_2\tilde{\phi}\big(\tilde{A}\otimes I_n\big)D_3\tilde{g}\right)^{-1}\end{bmatrix}
$$

with $\tilde{0}^1 = (\tilde{0}_1)^T = \underbrace{(0,...,0)}_{s-1}$.

We can now insert this back into ΔY and obtain:

$$
\begin{aligned}
\Delta Y =&\Delta\eta + h\delta_Y + h\begin{pmatrix}A & \\ \hat{A} & \end{pmatrix}\left(D_yF\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right) \\
&-\begin{pmatrix}A & \\ \hat{A} & \end{pmatrix}D_\lambda\tilde{F}\begin{pmatrix}0 & \\ (D_2\phi AD_3g)^- & \end{pmatrix} \\
&\times\left\{D_y\phi\left[\Delta\eta + h\delta_y + h\begin{pmatrix}A & \\ A & \end{pmatrix}\left(D_yF\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right)\right] + \theta\right\}.
\end{aligned}
\tag{5.18}
$$

Introducing the projectors:

$$
\begin{aligned}
\Pi_{\hat{A}}^A :=& I - \begin{pmatrix}A & \\ \hat{A} & \end{pmatrix}D_\lambda\tilde{F}\begin{pmatrix}0 & \\ (D_2\phi AD_3g)^- & \end{pmatrix}D_y\phi \\
P_A :=& I - D_\lambda\tilde{F}\begin{pmatrix}0 & \\ (D_2\phi AD_3g)^- & \end{pmatrix}D_y\phi\begin{pmatrix}A & \\ A & \end{pmatrix}.
\end{aligned}
$$

this expression can be further simplified as:

$$
\begin{aligned}
\Delta Y =&\Pi_{\hat{A}}^A\left(\Delta\eta + h\delta_y\right) + h\begin{pmatrix}A & \\ \hat{A} & \end{pmatrix}P_A\left(D_yF\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right) \\
&-\begin{pmatrix}A & \\ \hat{A} & \end{pmatrix}D_\lambda\tilde{F}\begin{pmatrix}0 & \\ (D_2\phi AD_3g)^- & \end{pmatrix}\theta + h\left(\delta_Y - \delta_y\right)
\end{aligned}
\tag{5.19}
$$

As for Δy, we have:

$$
\begin{aligned}
\Delta y =&\Delta\eta + h\delta_y + h\begin{pmatrix}A & \\ A & \end{pmatrix}\left(D_yF\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right) \\
&-\begin{pmatrix}A & \\ A & \end{pmatrix}D_\lambda\tilde{F}\begin{pmatrix}0 & \\ (D_2\phi AD_3g)^- & \end{pmatrix} \\
&\times\left\{D_y\phi\left[\Delta\eta + h\delta_y + h\begin{pmatrix}A & \\ A & \end{pmatrix}\left(D_yF\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right)\right] + \theta\right\}
\end{aligned}
\tag{5.20}
$$

which, using $\Pi_A := \Pi_A^A$, can be simplified as:

$$
\begin{aligned}
\Delta y =&\Pi_A\left[\Delta\eta + h\delta_y + h\begin{pmatrix}A & \\ A & \end{pmatrix}\left(D_yF\Delta Y + D_\lambda F_1\Delta\Lambda_0^1\right)\right] \\
&-\begin{pmatrix}A & \\ A & \end{pmatrix}D_\lambda\tilde{F}\begin{pmatrix}0 & \\ (D_2\phi AD_3g)^- & \end{pmatrix}\theta.
\end{aligned}
\tag{5.21}
$$

From eqs.(5.19) and (5.21) we can derive the result of the theorem almost directly. The trickiest term, $h^2\left\|\Delta\lambda_0\right\|$ in $\left\|\Delta p_i\right\|$, is the one already derived by Jay in [Jay93]. Reading

off the terms directly seems to point towards $h\left\|\Delta\lambda_0\right\|$, but this estimation can be refined as follows. Realise that:

$$\begin{aligned}\Pi_A &= \begin{bmatrix} 1\otimes I_n & 0 & 0 & 0 \\ 0 & I_{s-1}\otimes I_n & 0 & 0 \\ 0 & 0 & 1\otimes I_n & 0 \\ 0 & -\left(\tilde{A}\otimes I_n\right)\tilde{X}_1 & 0 & I_{s-1}\otimes I_n - \left(\tilde{A}\otimes I_n\right)\tilde{X}_2 \end{bmatrix} \\ &= \begin{bmatrix} 1\otimes I_n & 0 & 0 & 0 \\ 0 & I_{s-1}\otimes I_n & 0 & 0 \\ 0 & 0 & 1\otimes I_n & 0 \\ 0 & \tilde{\Pi}_{1,A} & 0 & \tilde{\Pi}_{2,A} \end{bmatrix}\end{aligned} \tag{5.22}$$

with:

$$\begin{aligned}\tilde{X}_i :=& D_3\tilde{g}\left(D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right)D_3\tilde{g}\right)^{-1}D_i\tilde{\phi} \\ =& D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1}\left(D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right)D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1}\right)^{-1}D_i\tilde{\phi}\end{aligned} \tag{5.23}$$

where in the second line we have inserted the identity matrix as $I_{s-1} = \tilde{A}^{-1}\tilde{A}$.

One can easily check that $\tilde{\Pi}_{2,A}\left(\tilde{A}\otimes I_n\right)D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1} = 0$. Now, the non-zero components of $h\Pi_A\begin{pmatrix}A \\ A\end{pmatrix}D_\lambda F_1\Delta\Lambda_0^1$ are $h\tilde{\Pi}_{2,A}D_3g_1\left(\tilde{A}_1\otimes\Delta\Lambda_0^1\right)$. Thus, we can finally write:

$$\begin{aligned}&h\tilde{\Pi}_{2,A}\left(\left(\tilde{A}\otimes I_n\right)D_3\tilde{g}\left(\tilde{A}\otimes I_n\right)^{-1} - D_3g_1\right)\left(\tilde{A}_1\otimes\Delta\Lambda_0^1\right) \\ &\quad= h\tilde{\Pi}_{2,A}\mathcal{O}(h)\left(\tilde{A}_1\otimes\Delta\Lambda_0^1\right) \\ &\quad= \mathcal{O}\left(h^2\left\|\Delta\lambda_0\right\|\right).\end{aligned} \tag{5.24}$$

This cannot be done for $\|\Delta P_0^i\|$, which makes it $\mathcal{O}\left(h\left\|\Delta\lambda_0\right\|\right)$. Inserting this back into either ΔY or Δy confirms that $\|\Delta Q_0^i\|$ is $\mathcal{O}\left(h^2\left\|\Delta\lambda_0\right\|\right)$. □

Lemma 5.2.3. *In addition to the hypotheses of theorem 5.2.1, suppose that $C(q)$, $\hat{C}(\hat{q})$ and $C\hat{C}(Q)$ and that $(D_1\phi\cdot f)(q_0,p_0)+(D_2\phi\cdot g)(q_0,p_0,\lambda_0)=\mathcal{O}(h^\kappa)$, with $\kappa\geq 1$. Then the solution of eq.*(5.13)*, Q_0^i, p_0^i, P_0^i and Λ_0^i satisfies:*

$$\begin{aligned}Q_0^i &= q_0 + \sum_{j=1}^{\lambda}\frac{c_i^jh^j}{j!}DQ_0^{(j)}(q_0,p_0) + \mathcal{O}(h^{\lambda+1}) \\ p_0^i &= p_0 + \sum_{j=1}^{\lambda}\frac{c_i^jh^j}{j!}DP_0^{(j)}(q_0,p_0,\lambda_0) + \mathcal{O}(h^{\lambda+1}) \\ P_0^i &= p_0 + \sum_{j=1}^{\mu}\frac{c_i^jh^j}{j!}DP_0^{(j)}(q_0,p_0,\lambda_0) + \mathcal{O}(h^{\mu+1}) \\ \Lambda_0^i &= \lambda_0(q_0,p_0) + \sum_{j=1}^{\nu}\frac{c_i^jh^j}{j!}D\Lambda_0^{(j)}(q_0,p_0,\lambda_0) + \mathcal{O}(h^{\nu+1})\end{aligned}$$

where $\lambda_0(q_0,p_0)$ is implicitly defined by the condition $(D_1\phi\cdot f)(q_0,p_0)+(D_2\phi\cdot g)(q_0,p_0,\lambda_0(q_0,p_0))=0$, $\lambda=\min(\kappa+1,q,\max(\hat{q}+1,Q+1))$, $\mu=\min(\kappa,\hat{q})$, $\nu=\min(\kappa-1,q-1)$, and $DQ_0^{(i)}$, $DP_0^{(i)}$ and $D\Lambda_0^{(i)}$ are functions composed by the derivatives of f, g and ϕ evaluated at $(q_0,p_0,\lambda_0(q_0,p_0))$.

Proof. Following [Jay93, Lemma 4.3] we can use the implicit function theorem to obtain $\lambda_0(q_0, p_0) - \lambda_0 = \mathcal{O}(h^\kappa)$. Assume $(q(t), p(t), \lambda(t))$ is the exact solution of eq.(5.6) with $q(t_0) = q_0$, $p(t_0) = p_0$ and $\lambda(t_0) = \lambda_0$, and let $Q_0^i = q(t_0 + c_i h)$, $p_0^i = P_0^i = p(t_0 + c_i h)$ and $\Lambda_0^i = \lambda(t_0 + c_i h)$ in the result of theorem 5.16. Finally, let $\hat{Q}_0^i$, $\hat{p}_0^i$, $\hat{P}_0^i$ and $\hat{\Lambda}_0^i$ be the solution of eq.(5.15) with $\hat{q}_0 = q_0$, $\hat{p}_0 = p_0$, $\hat{\lambda}_0 = \lambda_0(q_0, p_0)$ and $\theta = 0$. As we satisfy the conditions of theorem 5.2.2 we are left with:

$$\begin{aligned}
\left\|\Delta Q_0^i\right\| &\leq C\left(h^{\kappa+2} + h\left\|\delta_Q\right\| + h^2\left\|\delta_p\right\| + h^2\left\|\delta_P\right\|\right) \\
\left\|\Delta p_0^i\right\| &\leq C\left(h^{\kappa+2} + h^2\left\|\delta_Q\right\| + h\left\|\delta_p\right\| + h^2\left\|\delta_P\right\|\right) \\
\left\|\Delta P_0^i\right\| &\leq C\left(h^{\kappa+1} + h^2\left\|\delta_Q\right\| + h\left\|\delta_p\right\| + h\left\|\delta_P\right\|\right) \\
\left\|\Delta \Lambda_0^i\right\| &\leq C\left(h^{\kappa} + \left\|\delta_Q\right\| + \left\|\delta_p\right\|\right)
\end{aligned}$$

where we have made use of the fact that $\|\Delta\lambda_0\| = \mathcal{O}(h^\kappa)$. What remains is to compute δ_Q, δ_p, δ_P to obtain the result we are after.

Inserting the exact solution into eq.(5.15) we obtain:

$$\begin{aligned}
q(t_0 + c_i h) &= q_0 + h\sum_{j=1}^{s} a_{ij} f(q(t_0 + c_j h), p(t_0 + c_j h)) + h\delta_{Q,i} \\
&= q_0 + h\sum_{j=1}^{s} a_{ij}\dot{q}(t_0 + c_i h) + h\delta_{Q,i} \\
p(t_0 + c_i h) &= p_0 + h\sum_{j=1}^{s} a_{ij} g(q(t_0 + c_j h), p(t_0 + c_j h), \lambda(t_0 + c_j h)) + h\delta_{p,i} \\
&= p_0 + h\sum_{j=1}^{s} a_{ij}\dot{p}(t_0 + c_i h) + h\delta_{p,i} \\
p(t_0 + c_i h) &= p_0 + h\sum_{j=1}^{s} \hat{a}_{ij} g(q(t_0 + c_j h), p(t_0 + c_j h), \lambda(t_0 + c_j h)) + h\delta_{P,i} \\
&= p_0 + h\sum_{j=1}^{s} \hat{a}_{ij}\dot{p}(t_0 + c_i h) + h\delta_{P,i}
\end{aligned}$$

$$q(t_0 + c_i h) = q(t_0) + h\sum_{j=1}^{s} a_{ij} f(y(t_0 + c_j h), \lambda(t_0 + c_j h)) + h\delta_i\,.$$

Now, expanding in Taylor series about t_0 and taking into account that:

$$y(x_0 + c_i h) = y(x_0) + \sum_{j=1}^{m} \frac{1}{j!} y^{(j)}(x_0) c_i^j h^j + \mathcal{O}(h^{m+1})$$

we get:

$$\begin{aligned}
\delta_{Q,i} &= \frac{h^q q^{(q+1)}(x_0)}{q!}\left(\frac{c_i^{q+1}}{q+1} - \sum_{j=1}^{s} a_{ij} c_j^q\right) + \mathcal{O}(h^{q+1}) \\
\delta_{p,i} &= \frac{h^q p^{(q+1)}(x_0)}{q!}\left(\frac{c_i^{q+1}}{q+1} - \sum_{j=1}^{s} a_{ij} c_j^q\right) + \mathcal{O}(h^{q+1}) \\
\delta_{P,i} &= \frac{h^{\hat{q}} p^{(\hat{q}+1)}(x_0)}{\hat{q}!}\left(\frac{c_i^{\hat{q}+1}}{\hat{q}+1} - \sum_{j=1}^{s} \hat{a}_{ij} c_j^{\hat{q}}\right) + \mathcal{O}(h^{\hat{q}+1})\,.
\end{aligned}$$

Finally, we should be careful to note that according to eq.(5.21), $\delta_{P,i}$ enters in ΔQ_i and Δp_i multiplied by A so we may invoke $C\hat{C}(Q)$. Thus, we have:

$$\begin{aligned}\left\|\Delta Q_0^i\right\| &\leq C\left(h^{\min(\kappa+2,q+1,\max(\hat{q}+2,Q+2))}\right)\\ \left\|\Delta p_0^i\right\| &\leq C\left(h^{\min(\kappa+2,q+1,\max(\hat{q}+2,Q+2))}\right)\\ \left\|\Delta P_0^i\right\| &\leq C\left(h^{\min(\kappa+1,q+1,\hat{q}+1)}\right)\\ \left\|\Delta \Lambda_0^i\right\| &\leq C\left(h^{\min(\kappa,q)}\right)\end{aligned}$$

which proves our lemma. □

Remark. For the Lobatto IIIA-B methods we have that $\hat{q}+2 = Q = q = s$ and this result implies that:

$$\begin{aligned}\|\Delta Q_0^i\| &= \mathcal{O}(h^{\min(\kappa+2,s+1)}), \qquad \|\Delta P_0^i\| &= \mathcal{O}(h^{\min(\kappa+1,s-1)}),\\ \|\Delta p_0^i\| &= \mathcal{O}(h^{\min(\kappa+2,s+1)}), \qquad \|\Delta \Lambda_0^i\| &= \mathcal{O}(h^{\min(\kappa,s)}).\end{aligned}$$

△

For the development of the main theorem, on which the results of error and convergence rest, we will need the following definitions.

R-strings

Definition 5.2.1. (R-string). An R-string γ of dimension $\dim\gamma = s$ is an ordered list of s numbers $(\gamma_{(1)}, ..., \gamma_{(s)})$, where $\gamma_{(i)} \in \mathbb{N}_0$. $n = \max\gamma$ is said to be the order of the string.

Definition 5.2.2. (Irreducible R-string). An irreducible R-string γ of $\dim\gamma = s$, is such that for $1 < i < s$ even, $\gamma_{(i)}$ and $\gamma_{(i+1)}$ are not simultaneously zero.

For our purposes an R-string γ can be used as multi-index provided it is irreducible. They will appear in the terms:

$$R_\gamma = \tilde{C}^{\gamma_{(1)}}\tilde{A}^{-1}\left[\prod_{i\,\text{even}>0}^{\dim\gamma-2}\tilde{C}^{\gamma_{(i)}}\tilde{A}\tilde{C}^{\gamma_{(i+1)}}\tilde{A}^{-1}\right]\tilde{C}^{\gamma_{(\dim\gamma)}}$$

of a certain Taylor expansion which play an important role in the next theorem that we prove.

Let us define the following operations on these objects:

1. **Left appending.** Given an irreducible R-string γ of $\dim\gamma = s$ such that $\gamma_{(1)} \neq 0$, left appending gives a new R-string $\gamma' = (0, 0, \gamma_{(1)}, ..., \gamma_{s)})$ of $\dim\gamma' = s+2$.

2. **Right appending.** Given an irreducible R-string γ of $\dim\gamma = s$ such that $\gamma_{(s)} \neq 0$, right appending gives a new R-string $\gamma' = (\gamma_{(1)}, ..., \gamma_{(s)}, 0, 0)$ of $\dim\gamma' = s+2$.

3. **Insertion.** For $1 \leq i < s$ even, given an irreducible R-string γ such that $\gamma_{(i)} \neq 0 \neq \gamma_{(i+1)}$, insertion gives a new R-string

   $$\gamma' = (\gamma_{(1)}, ..., \gamma_{(i)}, 0, 0, \gamma_{(i+1)}, ..., \gamma_{(s)})$$

   of $\dim\gamma' = s+2$.

4. **Left splitting.** For $1 \leq i \leq s$, given an irreducible R-string γ such that $\gamma_{(i)} > 1$, left splitting gives a new R-string $\gamma' = (\gamma_{(1)}, ..., \gamma_{(i-1)}, 1, 0, \gamma_{(i)} - 1, ..., \gamma_{(s)})$ of $\dim \gamma' = s + 2$.

5. **Right splitting.** For $1 \leq i \leq s$, given an irreducible s-string γ such that $\gamma_{(i)} > 1$, right splitting gives a new R-string $\gamma' = (\gamma_{(1)}, ..., \gamma_{(i)} - 1, 0, 1, \gamma_{(i+1)}, ..., \gamma_{(s)})$ of $\dim \gamma' = s + 2$.

6. **Capping.** Given an irreducible s-string γ such that $\gamma_{(1)} \neq 0 \neq \gamma_{(s)}$, capping gives a new R-string $\gamma' = (0, \gamma_{(1)}, ..., \gamma_{(s)}, 0)$ of $\dim \gamma' = s + 2$.

7. **Left Diffusion.** For $1 < i \leq s$, given an irreducible s-string γ such that $\gamma_{(i)} > 1$, diffusion gives a new R-string $\gamma' = (\gamma_{(1)}, ..., \gamma_{(i-1)} + 1, \gamma_{(i)} - 1, ..., \gamma_{(s)})$ of $\dim \gamma' = s$.

8. **Right Diffusion.** For $1 \leq i < s$, given an irreducible s-string γ such that $\gamma_{(i)} > 1$, diffusion gives a new R-string $\gamma' = (\gamma_{(1)}, ..., \gamma_{(i)} - 1, \gamma_{(i+1)} + 1, ..., \gamma_{(s)})$ of $\dim \gamma' = s$.

All of these operations preserve irreducibility. Note that insertion can be absorbed into the splitting operations if we let $\gamma_{(i)} \geq 1$, but then we would need to add provisions so that the extended splitting operations preserve irreducibility.

Definition 5.2.3. (R-string class). We say that given two irreducible R-strings γ and δ, with $|\gamma| = |\delta|$ but $\dim \gamma$ and $\dim \delta$ not necessarily equal, are in the same *class* iff $R_\gamma = R_\delta$.

If two strings belong to the same class, then one can be derived from the other following certain rules. For a given order there are as many unique R coefficients as *elementary R-strings*.

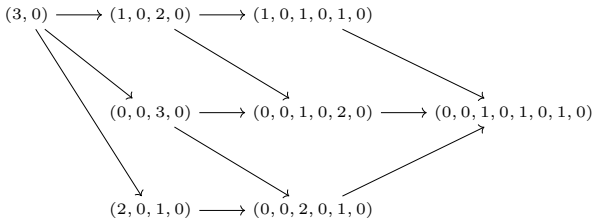
Definition 5.2.4. (Elementary R-string). An elementary string of order n is the shortest irreducible R-string of even dimension such that it cannot be derived from another elementary R-string via splitting, appending or insertion.

The n-th order has 2^n elementary strings. The simplest elementary R-strings of a given order are of dimension 2, i.e. R-strings $\gamma = (\gamma_{(1)}, \gamma_{(2)})$ such that $\gamma_{(1)} + \gamma_{(2)} = n$, of which there are $n + 1$. The rest of the elementary strings can be obtained from these via diffusion and capping.

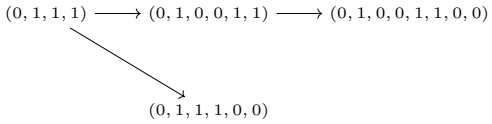
For $n = 3$, we know there are $2^3 = 8$ elementary R-strings. We have the following elementary R-strings of dimension 2: $(0, 3)$, $(1, 2)$, $(2, 1)$, $(3, 0)$. We may obtain the remaining four by capping and diffusion. First, we may cap $(1, 2)$ and $(2, 1)$ to obtain $(0, 1, 2, 0)$ and $(0, 2, 1, 0)$ respectively. From these new elementary R-strings of dimension 4 we obtain $(0, 1, 1, 1)$ and $(1, 1, 1, 0)$.

For $n = 4$, we know there are $2^4 = 16$ elementary strings. We have the following elementary R-strings of dimension 2: $(0, 4)$, $(1, 3)$, $(2, 2)$, $(3, 1)$, $(4, 0)$. First, we may cap $(1, 3)$, $(2, 2)$ and $(3, 1)$ to obtain $(0, 1, 3, 0)$, $(0, 2, 2, 0)$ and $(0, 3, 1, 0)$ respectively. From these new elementary R-strings we obtain $(0, 1, 3, 0)$, $(0, 1, 2, 1)$, $(0, 1, 1, 2)$, $(0, 2, 2, 0)$, $(1, 1, 1, 1)$, $(1, 2, 1, 0)$, $(2, 1, 1, 0)$. Finally, we may cap again the only R-string of dimension 4 that admits capping, $(1, 1, 1, 1)$, obtaining $(0, 1, 1, 1, 1, 0)$.

Example 5.2.1. As an example of derivation of strings of a class, let us take $(3, 0)$. Applying the left appending operation we can obtain $(0, 0, 3, 0)$. Applying the splitting operation to $(3, 0)$ we obtain $(2, 0, 1, 0)$ and $(1, 0, 2, 0)$. The rest of the derived strings of the class can be obtained via further appending and/or splitting: $(0, 0, 2, 0, 1, 0)$, $(0, 0, 1, 0, 2, 0)$, $(1, 0, 1, 0, 1, 0)$ and $(0, 0, 1, 0, 1, 0, 1, 0)$.



Example 5.2.2. Another example where we may use insertion is $(0, 1, 1, 1)$, which yields $(0, 1, 0, 0, 1, 1)$. The rest of the elements of the class are obtained via appending $(0, 1, 1, 1, 0, 0)$ and $(0, 1, 0, 0, 1, 1, 0, 0)$.



Theorem 5.2.4. *In addition to the hypotheses of theorem 5.2.2, suppose that A and $\hat{A}$ are symplectically conjugated and, $C(q)$, $\hat{C}(r)$, $D(r)$, $\hat{D}(q)$, $D\hat{D}(p-r)$, $\hat{D}D(p-q)$ and H3 hold. Furthermore, $(D_1\phi \cdot f)(q_0, p_0) + (D_2\phi \cdot g)(q_0, p_0, \lambda_0) = \mathcal{O}(h^\kappa)$, with $\kappa \geq 1$. Then we have:*

$$\begin{aligned} \|\Delta Q_0^s\| &= \Delta q_0 \\ &\quad + \mathcal{O}\left(h\|\Delta p_0\| + h^{m+2}\|\Delta\lambda_0\| + h\|\delta_Q\| + h^2\|\delta_p\| + h^2\|\delta_P\| + h\|\theta\|\right) \end{aligned} \tag{5.25}$$

$$\begin{aligned} \|\Delta p_0^s\| &= \Pi_{1,0}(q_0, p_0, \lambda_0)\Delta q_0 + \Pi_{2,0}(q_0, p_0, \lambda_0)\Delta p_0 \\ &\quad + \mathcal{O}\left(h^{m+2}\|\Delta\lambda_0\| + h^2\|\delta_Q\| + h\|\delta_p\| + h^2\|\delta_P\| + \|\theta\|\right) \end{aligned} \tag{5.26}$$

$$\begin{aligned} \|\Delta\Lambda_0^s\| &= \mathcal{R}_A(\infty)\Delta\lambda_0 \\ &\quad + \mathcal{O}\left(\|\Delta q_0\| + \|\Delta p_0\| + h\|\Delta\lambda_0\| + \|\delta_Q\| + \|\delta_p\| + \|\theta\|/h\right) \end{aligned} \tag{5.27}$$

where $m = \min(\kappa - 1, q - 1, r, p - q, p - r)$, $\mathcal{R}_A$ is the stability function of the method A, $\Pi_{1,0} = -D_3g(D_2\phi D_3g)D_1\phi$ and $\Pi_{2,0} = I_n - D_3g(D_2\phi D_3g)D_2\phi$.

Proof. This proof follows closely that of [Jay93, theorem 4.4]. The idea is to take the results from theorem 5.2.2 and perform a Taylor expansion of each term, focusing on the s-th component. Just as in [Jay93], the important result here is the h^{m+2} factor in front of $\|\Delta\lambda_0\|$, which means that we need to pay special attention to $\Delta\Lambda_0^1$.

In our case $\Delta\Lambda_0^s$ coincides with ΔZ_s in [Jay93] of the same theorem without changes. The differences appear in the rest of the components, where having two sets of Runge-Kutta coefficients makes the Taylor expansion of the terms and the tracking of each component much more difficult. We want ΔQ_0^s and Δp_0^s, as ΔP_0^s is not an external stage / nodal value. Thus, we will need to expand eq.(5.21). This depends on eq.(5.19), making it more challenging. Let us first solve this latter equation for ΔY:

$$\begin{aligned} \Delta Y = &\left(I - h\begin{pmatrix} A & \\ & \hat{A} \end{pmatrix} P_A D_y F\right)^{-1} \\ &\times \Big[\Pi_{\hat{A}}^A(\Delta\eta + h\delta_y) + h\begin{pmatrix} A & \\ & \hat{A} \end{pmatrix} P_A D_\lambda F_1 \Delta\Lambda_0^1 \\ &- \begin{pmatrix} A & \\ & \hat{A} \end{pmatrix} D_\lambda \tilde{F} \begin{pmatrix} 0 & \\ & (D_2\phi A D_3 g)^- \end{pmatrix} \theta + h(\delta_Y - \delta_y)\Big] . \end{aligned}$$

We then need to insert this in eq.(5.21). From here on we will forget about all terms except for the ones with $\Delta\Lambda_0^1$, as the rest vary little from what was found in Theorem

5.2.2 and they can be easily obtained, thus barring the need to carry them around any longer.

$$\begin{aligned}\Delta y = & h\Pi_A \begin{pmatrix} A \\ A \end{pmatrix} D_\lambda F_1 \Delta\Lambda_0^1 \\ & + h^2 \Pi_A \begin{pmatrix} A \\ A \end{pmatrix} D_y F \left(I - h \begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_y F\right)^{-1} \begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_\lambda F_1 \Delta\Lambda_0^1 \\ & + \ldots\end{aligned}$$

The first term can be expanded just as in [Jay93], as there is no $\hat{A}$ involved, giving us $\mathcal{O}(h^{m+2}\,\|\Delta\lambda_0\|)$ as expected. The second term is where the real changes appear. Let us begin with the right-most part of the term, $\begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_\lambda F_1 \Delta\Lambda_0^1$. We have that:

$$P_A = \begin{bmatrix} 1\otimes I_n & 0 & 0 & 0 \\ 0 & I_{s-1}\otimes I_n & 0 & 0 \\ 0 & 0 & 1\otimes I_n & 0 \\ -\tilde{X}_1\big(\tilde{A}_1\otimes I_n\big) & -\tilde{X}_1\big(\tilde{A}\otimes I_n\big) & -\tilde{X}_2\big(\tilde{A}_1\otimes I_n\big) & I_{s-1}\otimes I_n - \tilde{X}_2\big(\tilde{A}\otimes I_n\big) \end{bmatrix}$$

where $\tilde{X}_i$ was already defined in eq.(5.23) and where we have used the fact that a_{11} is zero and $\tilde{A}^1$ is a zero vector.

For the product $P_A D_\lambda F_1 \Delta\Lambda_0^1$ we only need to worry about the components $1\otimes I_n$ and $-\tilde{X}_2\left(\tilde{A}_1\otimes I_n\right)$, as the rest do not connect with $\Delta\Lambda_0^1$:

$$\begin{aligned}\begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_\lambda F_1 \Delta\Lambda_1 = & \begin{bmatrix} a_{11}\otimes I_n & \tilde{A}^1\otimes I_n & 0 & 0 \\ \tilde{A}_1\otimes I_n & \tilde{A}\otimes I_n & 0 & 0 \\ 0 & 0 & \hat{a}_{11}\otimes I_n & \hat{\tilde{A}}^1\otimes I_n \\ 0 & 0 & \hat{\tilde{A}}_1\otimes I_n & \hat{\tilde{A}}\otimes I_n \end{bmatrix} \\ \times & \begin{bmatrix} 1\otimes I_n & 0 & 0 & 0 \\ 0 & I_{s-1}\otimes I_n & 0 & 0 \\ 0 & 0 & 1\otimes I_n & 0 \\ -\tilde{X}_1\big(\tilde{A}_1\otimes I_n\big) & -\tilde{X}_1\big(\tilde{A}\otimes I_n\big) & -\tilde{X}_2\big(\tilde{A}_1\otimes I_n\big) & I_{s-1}\otimes I_n - \tilde{X}_2\big(\tilde{A}\otimes I_n\big) \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ D_3\tilde{g}_0\Delta\Lambda_0^1 \\ 0 \end{bmatrix}.\end{aligned} \tag{5.28}$$

Inside $\tilde{X}_2$, we find the product $D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right) D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1}$ composed of:

$$D_2\tilde{\phi} = \sum_{i=0}^{\omega} h^i \tilde{C}^i \otimes D_2\tilde{\phi}_i + \mathcal{O}(h^{\omega+1})$$

$$\left(\tilde{A}\otimes I_n\right) D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1} = \sum_{i=0}^{\omega} h^i \tilde{A}\tilde{C}^i\tilde{A}^{-1} \otimes D_3\tilde{g}_i + \mathcal{O}(h^{\omega+1})$$

which results in:

$$D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right) D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1} = \sum_{0\le i+j\le\omega} h^{i+j}\tilde{C}^i\tilde{A}\tilde{C}^j\tilde{A}^{-1} \otimes D_2\tilde{\phi}_i D_3\tilde{g}_j + \mathcal{O}(h^{\omega+1}).$$

Inversion of this product can be carried out as a Taylor expansion resulting in a so-

called von Neumann series $(I-T)^{-1} = \sum_{i=0}^{\infty} T^i$. Let us rewrite the former expression:

$$
\begin{aligned}
& D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right) D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1} \\
&= \left(I_{s-1}\otimes I_n + \sum_{1<i+j\leq\omega}^{\omega} h^{i+j}\tilde{C}^i\tilde{A}\tilde{C}^j\tilde{A}^{-1}\otimes D_2\tilde{\phi}_i D_3\tilde{g}_j\left(D_2\tilde{\phi}_0 D_3\tilde{g}_0\right)^{-1}\right) \\
&\times \left(I_{s-1}\otimes D_2\tilde{\phi}_0 D_3\tilde{g}_0\right) + \mathcal{O}(h^{\omega+1}) \\
&= \left(I_{s-1}\otimes I_n + \sum_{1<i+j\leq\omega}^{\omega} h^{i+j}\tilde{C}^i\tilde{A}\tilde{C}^j\tilde{A}^{-1}\otimes D_2\tilde{\phi}_i D_3\tilde{g}_j\ \triangle\right) \\
&\times (I_{s-1}\otimes\nabla) + \mathcal{O}(h^{\omega+1}) \\
&= \left(I_{s-1}\otimes I_n - \sum_{1<|\alpha|}^{\omega} -h^{|\alpha|}N_\alpha\otimes M_\alpha\right)\times(I_{s-1}\otimes\nabla) + \mathcal{O}(h^{\omega+1})
\end{aligned}
$$

with α multi-index of $\dim\alpha = 2$. For instance, for $|\alpha| = 3$ we have $\alpha_1 = (3,0), \alpha_2 = (2,1), \alpha_3 = (1,2), \alpha_1 = (0,3)$, and the corresponding terms $N_\alpha\otimes M_\alpha$ are:

$$
\begin{aligned}
N_{(3,0)}\otimes M_{(3,0)} &= \tilde{C}^3\otimes D_2\tilde{\phi}_3 D_3\tilde{g}_0\ \triangle \\
N_{(2,1)}\otimes M_{(2,1)} &= \tilde{C}^2\tilde{A}\tilde{C}\tilde{A}^{-1}\otimes D_2\tilde{\phi}_2 D_3\tilde{g}_1\ \triangle \\
N_{(1,2)}\otimes M_{(1,2)} &= \tilde{C}\tilde{A}\tilde{C}^2\tilde{A}^{-1}\otimes D_2\tilde{\phi}_1 D_3\tilde{g}_2\ \triangle \\
N_{(0,3)}\otimes M_{(0,3)} &= \tilde{A}\tilde{C}^3\tilde{A}^{-1}\otimes D_2\tilde{\phi}_0 D_3\tilde{g}_3\ \triangle\ .
\end{aligned}
$$

We have also made use of the short-hand notation $\nabla = D_2\tilde{\phi}_0 D_3\tilde{g}_0$ and $\triangle = \left(D_2\tilde{\phi}_0 D_3\tilde{g}_0\right)^{-1}$.

Paying attention to the non-commutativity of the series we obtain:

$$
\begin{aligned}
& \left(D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right) D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1}\right)^{-1} \\
&= (I_{s-1}\otimes\ \triangle)\times\left(\sum_{|\beta|=0}^{\omega}(-1)^{\frac{\dim\beta}{2}}h^{|\beta|}N_\beta\otimes M_\beta\right) + \mathcal{O}(h^{\omega+1})
\end{aligned}
$$

with β multi-index of $\dim\beta \leq 2\omega$, even, and such that for i *odd* $\beta_{(i)}$ and $\beta_{(i+1)}$ are never both 0. For instance, for $|\beta| = 2$ and $\dim\beta = 2$, we have $\beta_{1,1} = (2,0), \beta_{1,2} = (1,1), \beta_{1,3} = (0,2)$, and for $\dim\beta = 4$, we have $\beta_{2,1} = (1,0,1,0), \beta_{2,2} = (1,0,0,1), \beta_{2,3} = (0,1,1,0), \beta_{2,4} = (0,1,0,1)$. $(0,0,1,1)$ and $(1,1,0,0)$ are not allowed as they contain two contiguous zeros in odd and even position. Some examples of the corresponding terms $N_\beta\otimes M_\beta$ are:

$$
\begin{aligned}
N_{(1,1)}\otimes M_{(1,1)} &= \tilde{C}\tilde{A}\tilde{C}\tilde{A}^{-1}\otimes D_2\tilde{\phi}_1 D_3\tilde{g}_1\ \triangle \\
N_{(0,1,1,0)}\otimes M_{(0,1,1,0)} &= \tilde{A}\tilde{C}\tilde{A}^{-1}\tilde{C}\otimes D_2\tilde{\phi}_0 D_3\tilde{g}_1\ \triangle\ D_2\tilde{\phi}_1 D_3\tilde{g}_0\ \triangle\ .
\end{aligned}
$$

We need to include the restriction on elements such as $(0,0,1,1)$ as a double-counting prevention of sorts. We can understand this by checking what its associated $M_{(0,0,1,1)}$ would look like:

$$
D_2\tilde{\phi}_0 D_3\tilde{g}_0\ \triangle\ D_2\tilde{\phi}_1 D_3\tilde{g}_1\ \triangle = \nabla\ \triangle\ D_2\tilde{\phi}_1 D_3\tilde{g}_1\ \triangle = D_2\tilde{\phi}_1 D_3\tilde{g}_1\ \triangle = M_{(1,1)}\ .
$$

Moving on to the next computation, we sandwich the expression between $D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)$ and $D_2\tilde{\phi}$ to obtain:

$$\begin{aligned}\tilde{X}_2 &= D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)\left(D_2\tilde{\phi}\left(\tilde{A}\otimes I_n\right)D_3\tilde{g}\left(\tilde{A}\otimes I_m\right)^{-1}\right)^{-1}D_2\tilde{\phi}\\ &= \left(\sum_{|\gamma|=0}^{\omega}(-1)^{\frac{\dim\gamma}{2}-1}h^{|\gamma|}R_\gamma\otimes S_\gamma\right)+\mathcal{O}(h^{\omega+1})\end{aligned}$$

where:

$$\begin{aligned}R_\gamma &= \tilde{C}^{\gamma_{(1)}}\tilde{A}^{-1}\left[\prod_{i\,\text{even}>0}^{\dim\gamma-2}\tilde{C}^{\gamma_{(i)}}\tilde{A}\tilde{C}^{\gamma_{(i+1)}}\tilde{A}^{-1}\right]\tilde{C}^{\gamma_{(\dim\gamma)}}\\ S_\gamma &= D_3\tilde{g}_{\gamma_{(1)}}\,\triangle\left[\prod_{i\,\text{even}>0}^{\dim\gamma-2}D_2\tilde{\phi}_{\gamma_{(i)}}D_3\tilde{g}_{\gamma_{(i+1)}}\,\triangle\right]D_2\tilde{\phi}_{\gamma_{(\dim\gamma)}}\end{aligned}$$

with γ multi-index of $\dim\gamma\le 2\omega$, even, and such that for i *even* $\gamma_{(i)}$ and $\gamma_{(i+1)}$ are never both 0, i.e. γ is an irreducible R-string.

This structure looks quite complicated as it is, and it does not seem to lend itself to easy groupings of symbol combinations R_γ. Nevertheless, it can be done with the help of the R-string classes we introduced before.

Once we have derived $\tilde{X}_2$ and essentially P_A, we can finally tackle the full product $\begin{pmatrix}A\\ \hat{A}\end{pmatrix}P_AD_\lambda F_1\Delta\Lambda_0^1$. If we perform the matrix multiplications in eq.(5.28) we get:

$$\begin{pmatrix}A\\ \hat{A}\end{pmatrix}P_AD_\lambda F_1\Delta\Lambda_0^1=\begin{bmatrix}0\\ 0\\ \hat{a}_{11}\otimes D_3\tilde{g}_0\Delta\Lambda_0^1-\left(\hat{\tilde{A}}^1\otimes I_n\right)\tilde{X}_2\left(\tilde{A}_1\otimes D_3\tilde{g}_0\Delta\Lambda_0^1\right)\\ \hat{\tilde{A}}_1\otimes D_3\tilde{g}_0\Delta\Lambda_0^1-\left(\hat{\tilde{A}}\otimes I_n\right)\tilde{X}_2\left(\tilde{A}_1\otimes D_3\tilde{g}_0\Delta\Lambda_0^1\right)\end{bmatrix}.$$

What is important here is that we are multiplying by $D_3\tilde{g}_0$ on the right. In terms of strings this means appending one zero to the right, which makes a big part of the expansion vanish, as we will see in proposition 5.2.1. This result gives us valuable information about the series expansion:

$$\left(\Pi_{A,0}+\mathcal{O}(h)\right)\begin{pmatrix}A\\ A\end{pmatrix}\left(D_yF_0+\mathcal{O}(h)\right)\left(I-\mathcal{O}(h)\right)^{-1}\begin{pmatrix}A\\ \hat{A}\end{pmatrix}P_AD_\lambda F_1\Delta\Lambda_0^1\,.$$

At order 0, for the last component we get that the combination

$$e_s^T\begin{bmatrix}a_{11}&\tilde{A}^1\\ \tilde{A}_1&\tilde{A}\end{bmatrix}\left(\begin{bmatrix}\hat{a}_{11}\\ \hat{\tilde{A}}_1\end{bmatrix}-\begin{bmatrix}\hat{\tilde{A}}^1\tilde{A}^{-1}\tilde{A}_1\\ \hat{\tilde{A}}\tilde{A}^{-1}\tilde{A}_1\end{bmatrix}\right)=0$$

where the vector $e_s^T=(0,...,0,1)$, with $\dim e_s=s$. For a method satisfying H3 we have that $e_s^TA=b$. Using the notation:

$$A^-=\begin{bmatrix}0&\tilde{0}^1\\ \tilde{0}_1&\tilde{A}^{-1}\end{bmatrix},\quad A_1=\begin{bmatrix}a_{11}\\ \tilde{A}_1\end{bmatrix},\quad \hat{A}_1=\begin{bmatrix}\hat{a}_{11}\\ \hat{\tilde{A}}_1\end{bmatrix}$$

we may write this expression in shorter form as $e_s^TA(\hat{A}_1-\hat{A}A^-A_1)$.

At order h we still do not have all the terms that arise from the expansion but we already have an interesting combination that must also vanish

$$e_s^T \begin{bmatrix} a_{11} & \tilde{A}^1 \\ \tilde{A}_1 & \tilde{A} \end{bmatrix} \begin{bmatrix} \hat{a}_{11} & \hat{\tilde{A}}^1 \\ \hat{\tilde{A}}_1 & \hat{\tilde{A}} \end{bmatrix} \begin{bmatrix} 0 \\ \tilde{C}\tilde{A}^{-1}\tilde{A}_1 \end{bmatrix} = 0\,.$$

We can write this combination as $e_s^T A\hat{A}CA^-A_1$.

In fact, the two vanishing combinations hint at the template for the rest of the vanishing combinations: $e_s^T \dots A \dots (\hat{A}_1 - \hat{A}A^-A_1)$ and $e_s^T \dots A \dots \hat{A} \dots CA^-A_1$.

As we will see later, for all combinations there will always be at least one $\hat{A}$ (which the first template already includes) and one A, as can be readily seen below:

$$\Pi_A \underline{\underline{\begin{pmatrix} A \\ A \end{pmatrix}}} D_y F \left(I - h \begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_y F\right)^{-1} \underline{\underline{\begin{pmatrix} A \\ \hat{A} \end{pmatrix}}} P_A D_\lambda F_1 \Delta\Lambda_0^1\,.$$

As we grow in order, up to order n, combinations of A, $\hat{A}$, C and A^-CA show up such that their number adds up to $n+1$. These originate from P_A itself, as well as Π_A, D_yF and $\left(I - h \begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_y F\right)^{-1}$, as we will soon see.

With all the knowledge we obtained from our string analysis, it can be shown that the expansion of $\begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_\lambda F_1 \Delta\Lambda_0^1$ takes the form:

$$\begin{aligned} &(\hat{A}_1 - \hat{A}A^-A_1) \otimes D_3 g_0 \Delta\Lambda_0^1 \\ &+ \sum_{|\rho|=0}^{\omega} h^{|\rho|+1} \left[\hat{A} \left(\prod_{i\,\mathrm{odd}\geq 1}^{\dim\rho-1} C^{\rho(i)} A^- C^{\rho(i+1)} A \right) C \otimes O_\rho \Delta\Lambda_0^1 \right] + \mathcal{O}(h^{\omega+1}) \end{aligned}$$

where O_ρ is a term composed by multiplication of $\triangle$ and derivatives of g and ϕ evaluated at the initial condition.

For the remaining expansions we do not need to be as precise as with this last one as there will not be cancellations due to signs. Thus, we will only care about the different symbol combinations that arise.

The object $\left(I - h \begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_y F\right)^{-1}$ is the most involved of all of them as it is a matrix term that couples the ΔQ_0 and ΔP_0 equations. The matrix multiplied by h is:

$$\begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_y F = \begin{bmatrix} AD_1 f & AD_2 f \\ -\hat{A}[D_1 f X_1 A + D_1 g(X_2 A - \mathbb{1})] & -\hat{A}[D_2 f X_1 A + D_2 g(X_2 A - \mathbb{1})] \end{bmatrix}.$$

If we write $I - h \begin{pmatrix} A \\ \hat{A} \end{pmatrix} P_A D_y F$ as:

$$\begin{bmatrix} 1-K & -L \\ -M & 1-N \end{bmatrix}$$

where the matrices K, L, M, N are $\mathcal{O}(h)$, then its inverse must be:

$$\begin{bmatrix} W & X \\ Y & Z \end{bmatrix}$$

with:

$$\begin{aligned} W &= (1 - K - L(1-N)^{-1}M)^{-1}, \\ X &= (1-K)^{-1}L(1 - N - M(1-K)^{-1}L)^{-1}, \\ Y &= (1-N)^{-1}M(1 - K - L(1-N)^{-1}M)^{-1}, \\ Z &= (1 - N - M(1-K)^{-1}L)^{-1}. \end{aligned}$$

The only terms we are interested in are X and Z, as those are the only ones that connect with $\Delta\Lambda_1$. The Taylor expansion of any of these terms is a daunting task given the amount of nested expansions of non-commutative terms involved. Instead, we deem it sufficient to analyze the symbolic expansion found via CAS up to order 4 and draw our conclusions from there. In our case we will use the SymPy library for Python for the actual computations.

Before we begin analyzing terms, it is interesting to check the form of X and Z. We can see that $X = (1 - K)^{-1}LZ$. This means that once we know the behavior of Z, the behavior of X will be easy to derive. Also from this, we can easily see that all the resulting symbol combinations of X must necessarily start with the coefficient matrix A, while for Z they must start with the coefficient matrix $\hat{A}$ with the exception of the zero-th order term. In fact, this is also true for W and Y respectively, being W the one with non-zero zero-th order term.

The expansion of Z (and Y) shows the following symbol combinations up to order 3:

Order	Term	1 Substitution	2 Substitutions
1	$\hat{A}$		
2	$\hat{A}A$		
	$\hat{A}C$	$\hat{A}A^{-}CA$	
	$\hat{A}^2$		
3	$\hat{A}A^2$		
	$\hat{A}AC$		
	$\hat{A}A\hat{A}$		
	$\hat{A}CA$	$\hat{A}A^{-}CA^2$	
	$\hat{A}C^2$	$\hat{A}A^{-}CAC$	$\hat{A}A^{-}C^2A$
		$\hat{A}CA^{-}CA$	
	$\hat{A}C\hat{A}$	$\hat{A}A^{-}CA\hat{A}$	
	$\hat{A}^2A$		
	$\hat{A}^2C$	$\hat{A}^2A^{-}CA$	
	$\hat{A}^3$		

As for the expansion of X (and W), we get:

Order	Term	1 Substitution	2 Substitutions
1	A		
2	A^2		
	AC		
	$A\hat{A}$		
3	A^3		
	A^2C		
	$A^2\hat{A}$		
	ACA		
	AC^2		
	$AC\hat{A}$		
	$A\hat{A}A$		
	$A\hat{A}C$	$A\hat{A}A^{-}CA$	
	$A\hat{A}^2$		

Focusing on Z, we can see that for order 2 we append either an A, C or $\hat{A}$ to the right of the order 1 terms. Also note that C can be substituted by the combination $A^{-}CA$ once, so long as the preceding symbol in the term without substitutions is not an A. We find the same relation between order 3 and order 2, and (although not shown here) for order 4 and order 3. Thus, the pattern of construction of terms to arbitrary order seems clear for Z.

Focusing now on X, and taking into account the discussion at the beginning of the section, we can see that all the terms in Z will show up multiplied by $(1-K)^{-1}L$. The symbols this factor adds at order n are $A \times [(n-1)$-element variations of $\{A, C\}]$. In practice, what we observe with the symbolic expansion is that every single term without substitution at order n in Z appears in X with the first $\hat{A}$ exchanged by A. As for substituted terms, at order n we find all substitution terms from Z up to order $n-1$ with a corresponding pre-factor $\{A, C\}$. For instance, if we take $\hat{A}A^{-}CA$, which is of order 2 for Z, we will find it as $A\hat{A}A^{-}CA$ at order 3, and as $AC\hat{A}A^{-}CA$ and $A^2\hat{A}A^{-}CA$ at order 4 and so on. An easier way to put this is that the construction of terms for X is the same as for Z with the restriction that substitutions $C \mapsto A^{-}CA$ can only appear after the first $\hat{A}$ that show up.

Let us finally expand the term $\Pi_A \begin{pmatrix} A & \\ & A \end{pmatrix} D_y F$. For the projector Π_A, (see eq.(5.22)), its $\tilde{\Pi}_{i,A}$ are very similar to the terms $\tilde{X}_i$ that we have already studied:

$$\tilde{\Pi}_{i,A} = \sum_{|\gamma|=0}^{\omega} h^{|\gamma|} \left[\prod_{j \text{ odd} \geq 1}^{\dim \gamma - 1} \tilde{C}^{\gamma_{(j)}} \tilde{A} \tilde{C}^{\gamma_{(j+1)}} \tilde{A}^{-1} \right] \otimes \tilde{\Pi}_{i,A,\gamma} + \mathcal{O}(h^{\omega+1}) \,.$$

It is important to note that as we have the product $\Pi_A \begin{pmatrix} A & \\ & A \end{pmatrix}$, we will always have one A^{-} less than the number of As, which prevents AC^kA^{-} terms from appearing at the very end of a symbol combination.

For the Jacobian $D_y F$ we have:

$$D_y F = \begin{bmatrix} D_1 f_1 & 0 & D_2 f_1 & 0 \\ 0 & D_1 \tilde{f} & 0 & D_2 \tilde{f} \\ D_1 g_1 & 0 & D_2 g_1 & 0 \\ 0 & D_1 \tilde{g} & 0 & D_2 \tilde{g} \end{bmatrix} = \begin{bmatrix} D_1 f & D_2 f \\ D_1 g & D_2 g \end{bmatrix} .$$

The expansion of each term follows the same pattern. For instance, for $D_2 g$ we have:

$$D_2 g = \sum_{i=0}^{\omega} h^i C^i \otimes D_2 g_i + \mathcal{O}(h^{\omega+1}) \,.$$

Considering all this, the product $\Pi_A \begin{pmatrix} A & \\ & A \end{pmatrix} D_y F$ has two differentiated symbol groupings: top row (corresponding to ΔQ) and bottom row (corresponding to Δp) groups.

Top row groups are the easiest ones as they are the ones that remain unaffected by Π_A. These are of the form:

$$\sum_{i=0}^{\omega} h^i \left[AC^i \otimes U_i \right] + \mathcal{O}(h^{\omega+1})$$

where U_i are linear combinations of derivatives of g and f evaluated at the initial condition. Bottom row groups show more variety. These are of the form:

$$\sum_{|\alpha|+|\beta|=0}^{\omega} h^{|\alpha|+|\beta|} \left[C^\alpha A \prod_{i \text{ odd} \geq 1}^{\dim \beta - 1} \left(C^{\beta_{(i)}} A^{-} C^{\beta_{(i+1)}} A \right) \otimes V_{\alpha,\beta} \right] + \mathcal{O}(h^{\omega+1})$$

where $V_{\alpha,\beta}$ are terms involving $\triangle$ and derivatives of f, g and ϕ evaluated at the initial condition. The main difference here is that bottom row terms can have Cs to the left of the first A, as well as the possibility of having $C \mapsto A^- CA$ substitutions to its right.

Putting everything together, and keeping in mind that $\omega = \min(\lambda, \mu, \nu)$, the expansion can be brought to the form:

$$\Delta Q = h^2 \sum_{i=0}^{m-1} h^i \left(\sum_{\alpha} K_{Q,\alpha_i} \otimes L_{Q,\alpha_i} \right) \Delta\Lambda_1 + \mathcal{O}(h^{m+2} \left\| \Delta\Lambda_0^1 \right\|)$$
$$\Delta p = h^2 \sum_{i=0}^{m-1} h^i \left(\sum_{\alpha} K_{p,\alpha_i} \otimes L_{p,\alpha_i} \right) \Delta\Lambda_1 + \mathcal{O}(h^{m+2} \left\| \Delta\Lambda_0^1 \right\|)$$

where each L_{j,α_i} is again a combination of products of the derivatives of f, g, ϕ with $\triangle$ evaluated at the initial condition, and K_{j,α_i} is a Runge-Kutta symbol combination of order $|\alpha_i|$ as in theorem 5.2.5. The difference between K_{Q,α_i} and K_{p,α_i} lies in the fact that K_{Q,α_i} cannot begin with C^i and there cannot be $C \mapsto A^- CA$ substitutions between the initial A and the first $\hat{A}$, while on K_{p,α_i} there can be. Applying the result of said theorem, all these terms vanish, which is what we set out to prove. □

Proposition 5.2.1. *In the Taylor expansion of $P_A D_\lambda F_1$ only the terms belonging to the classes with elementary R-strings with a trailing zero, i.e. γ R-strings of $\dim\gamma = s$ such that $\gamma_{(s)} = 0$, survive.*

Proof. Given a class with an elementary representative γ such that $\gamma_{(s)} \neq 0$ implies that it admits right appending, which gives us γ'. $R_\gamma = R_{\gamma'}$ by definition of class. On the other hand, $S_\gamma \neq S_{\gamma'}$ and $\dim\gamma' = \dim\gamma + 2$, which means both terms will have opposite signs. Now $S_{\gamma'} = S_\gamma D_3\tilde{g}_0 \triangle D_2\tilde{\phi}_0$, but $S_{\gamma'} D_3\tilde{g}_0 = S_\gamma D_3\tilde{g}_0 \triangle \nabla = S_\gamma D_3\tilde{g}_0$, which is exactly what we needed to show that they cancel each other out. This is also true for other elements derived from the same elementary R-string via splitting and insertion, as they still necessarily admit right appending. □

Theorem 5.2.5. *Assume an s-stage symplectic partitioned Runge-Kutta method with coefficients A satisfying hypotheses H1, H2, H3 (and consequently $\hat{A}$ satisfying H1' and H2'), together with conditions $D(r)$, $\hat{D}(q)$, $D\hat{D}(p-r)$ and $\hat{D}D(p-q)$. With $\alpha \geq 0$, we have:*

$$e_s^T C^\alpha A \left(\prod_{i=1}^{k} M_i \right) (\hat{A}_1 - \hat{A}A^- A_1) = 0, \quad 0 \leq k \leq \min(r, q, p-r, p-q) - 1 \tag{5.29}$$

and:

$$e_s^T C^\alpha A \left(\prod_{i=1}^{k} N_i \right) CA^- A_1, \quad 0 \leq k \leq \min(r, q, p-r, p-q) - 1 \tag{5.30}$$

where M_i and N_i can be C, A, $\hat{A}$, $A^- CA$, ACA^- for any i except k where $M_k = ACA^-$ cannot occur.

Proof. Multiplying $D(r)$ by A^- we may obtain that:

$$bC^k A^- = e_s^T - kbC^{k-1}, \quad 1 \leq k \leq r\,. \tag{5.31}$$

As A satisfies H3, we also have that $e_s^T A = b$, and consequently $bA^- = e_s^T$.

The vanishing of the different symbol terms rests in both the vanishing of the following reduced combinations and the fact that any symbol combination that appears in the expansion can be brought to one of these.

- Combination 1:

$$bC^{k-1}(\hat{A}_1 - \hat{A}A^-A_1) = 0, \quad 1 \le k \le \min(r, \hat{r})\,.$$

This is said to be of order $k-1$, as that is the number of times C appears. It vanishes because:

$$\begin{aligned} bC^{k-1}\hat{A}_1 &= k^{-1}b_1 \\ bC^{k-1}\hat{A}A^-A_1 &= k^{-1}b(1-C^k)A^-A_1 \\ &= k^{-1}bA^-A_1 - k^{-1}bC^kA^-A_1 \\ &= k^{-1}b_1 - k^{-1}\left(b_1 - kbC^{k-1}A_1\right) \\ &= k^{-1}b_1\,. \end{aligned}$$

The application of the simplifying assumption $\hat{D}(\hat{r})$ in the second line and $D(r)$ in the fourth line are the limiting factors.

- Combination 2:

$$bC^kA^-A_1 = 0, \quad 1 \le k \le r$$

This is said to be of order k, as that is the number of times C appears

$$\begin{aligned} bC^kA^-A_1 &= b_1 - kbC^{k-1}A_1 \\ &= b_1 - b_1 \\ &= 0\,. \end{aligned}$$

Again, the application of the simplifying assumption $D(r)$ in the first line is the limiting factor.

Combination 1 and combination 2 can be generalized to the form (5.29) and (5.30) respectively.

As $c_s = 1$, we have that $e_s^TC^\alpha = e_s^T$, thus the C^α is there only for generality. After recursive application of D, $\hat{D}$, $D\hat{D}$, $\hat{D}D$ and eq.(5.31), each of these expressions can be brought to a linear combination of one of the reduced combinations with different values of k, which proves the theorem. □

Remark. For an s-stage Lobatto III A-B method we have that $s-2 = r = p-q = q-2 = p-r-2$, thus:

$$e_s^TC^\alpha A\left(\prod_{i=1}^{k} M_i\right)(\hat{A}_1 - \hat{A}A^-A_1) = 0, \quad 0 \le k \le s-3 \tag{5.32}$$

$$e_s^TC^\alpha A\left(\prod_{i=1}^{k} N_i\right)CA^-A_1, \quad 0 \le k \le s-3\,. \tag{5.33}$$

△

Theorem 5.2.6. *Assume an s-stage symplectic partitioned Runge-Kutta method with coefficients A satisfying hypotheses H1, H2, H3 (and consequently $\hat{A}$ satisfying H1' and H2'), together with conditions $B(p)$, $C(q)$, $D(r)$ (and consequently $\hat{B}(p)$, $\hat{C}(r)$, $\hat{D}(q)$). Then we have:*

$$\delta q_h(x) = \mathcal{O}(h^{\min(p,q+r+1)+1}), \tag{5.34a}$$

$$\delta p_h(x) = \mathcal{O}(h^{\min(p,2q,q+r)+1}), \tag{5.34b}$$

$$\delta \lambda_h(x) = \mathcal{O}(h^q). \tag{5.34c}$$

Proof. The proof of this theorem is similar to that of [Jay93, theorem 5.1], which follows that of [HLR89, theorem 5.9], and [HW96, theorem 8.10].

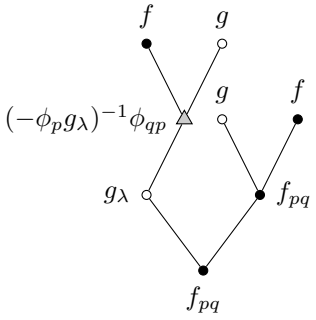


Figure 5.1: This order 6 tree represents the term $f_{pq}\left(g_\lambda(-\phi_p g_\lambda)^{-1}\phi_{qp}(f,g), f_{pq}(g,f)\right)$. Note that the order is derived from the number of round nodes minus the number of triangle nodes. The tree itself can be written as $[[[\tau_Q,\tau_P]_\lambda]_P,[\tau_P,\tau_Q]_Q]_Q$ and corresponds to the Runge-Kutta term: $b_i\hat{a}_{ij}a^-_{jk}c_k^2a_{il}c_l^2$, where a^-_{ij} are the components of the A^- matrix.

The arguments are essentially the same as those used in [HLR89] for A invertible, but using a bi-colored tree extension (see fig.5.1). The inverses that appear only need to be swapped by A^-. In these results two trees are used, t and u trees, referring to y and z equations respectively. In our case we will have both t_Q and t_P for Q and P equations, plus u for λ equations.

The key difference with respect to both this and Jay is that instead of only needing to set the limit such that for $[t,u]_y$ either t or u are above the maximum reduction order by $C(q)$ ($q+1$ and $q-1$), which leads to $2q$, we need to be careful because we have two types of trees with $C(q)$ and $\hat{C}(r)$. First of all, it is impossible to have $[t_Q,u]_Q$ as f does not depend on λ, and we can only have $[t_Q,t_P]_Q$, which pushes the limit to $q+r+2$. On the other hand, $[t_P,u]_P$ also sets a limit, which as it turns out is $q+r$. For both there is also the limit $q+r+1$ set by $D(r)$, which is more restrictive than the limit set for Q equations but less so than the limit set for P, so this last one prevails. □

Theorem 5.2.7. *Consider the IVP posed by the partitioned differential-algebraic system of eqs.*(5.6)*, together with consistent initial values and the Runge-Kutta method* (5.12)*. In addition to the hypotheses of theorem 5.2.6, suppose that* $\|R_A(\infty)\| \leq 1$ *and* $q \geq 1$ *if* $R_A(\infty)$*. Then, for* $t_n - t_0 = nh \leq C$*, where* C *is a constant, the global error satisfies:*

$$q_n - q(t_n) = \mathcal{O}(h^{\min(p,q+r+1)}) \tag{5.35a}$$

$$p_n - p(t_n) = \mathcal{O}(h^{\min(p,2q,q+r)}) \tag{5.35b}$$

$$\lambda_n - \lambda(t_n) = \begin{cases} \mathcal{O}(h^q) & \text{if } -1 \leq R_A(\infty) < 1, \\ \mathcal{O}(h^{q-1}) & \text{if } R_A(\infty) = 1. \end{cases} \tag{5.35c}$$

Proof. Following the steps of [Jay93, theorem 5.2], for $\|R(\infty)\| < 1$ and $\|R(\infty)\| = 1$, $\lambda_n - \lambda(t_n)$ can be found to be of order $\mathcal{O}(h^q)$ and $\mathcal{O}(h^{q-1})$ respectively. As stated there, the result for $R(\infty) = -1$ can actually be improved to $\mathcal{O}(h^q)$ by considering a perturbed asymptotic expansion.

Now, we proceed as in [HW96, theorem VI.7.5], applying (5.25)(5.26)(5.27) to two neighboring Runge-Kutta solutions, $\left\{\tilde{q}_n,\tilde{p}_n,\tilde{\lambda}_n\right\}$ and $\left\{\hat{q}_n,\hat{p}_n,\hat{\lambda}_n\right\}$, with $\delta_i = 0$, $\theta = 0$. Using the notation $\Delta x_n = \tilde{x}_n - \hat{x}_n$, we can write:

$$\begin{aligned}
\Delta q_{n+1} &= \Delta q_n + \mathcal{O}\left(h\|\Delta p_n\| + h^{m+2}\|\Delta\lambda_n\|\right) \\
\Delta p_{n+1} &= \Pi_{1,n}\Delta q_n + \Pi_{2,n}\Delta p_n + \mathcal{O}\left(h^{m+2}\|\Delta\lambda_n\|\right) \\
\Delta\lambda_{n+1} &= \mathcal{R}_A(\infty)\Delta\lambda_n + \mathcal{O}\left(\|\Delta q_n\| + \|\Delta p_n\| + h\|\Delta\lambda_n\|\right)
\end{aligned}$$

where $\Pi_{1,n}$ and $\Pi_{2,n}$ are the projectors defined in the statement of theorem 5.2.4, evaluated at $\hat{q}_n$, $\hat{p}_n$, $\hat{\lambda}_n$, and $m = \min(q-1, r, p-q, p-r)$ for $-1 \leq R(\infty) < 1$ or $m = \min(q-2, r, p-q, p-r)$ for $R(\infty) = 1$.

We can follow the same philosophy of [HLR89, lemma 4.5], and try to relate $\{\Delta q_n, \Delta p_n, \Delta\lambda_n\}$ with $\{\Delta q_0, \Delta p_0, \Delta\lambda_0\}$. For this, we make use of the fact that $\Pi_{i,n+1} = \Pi_{i,n} + \mathcal{O}(h)$, $(\Pi_{2,k})^2 = \Pi_{2,k}$ and $\Pi_{2,k}\Pi_{1,k} = 0$ (these latter facts can be readily derived from their definition).

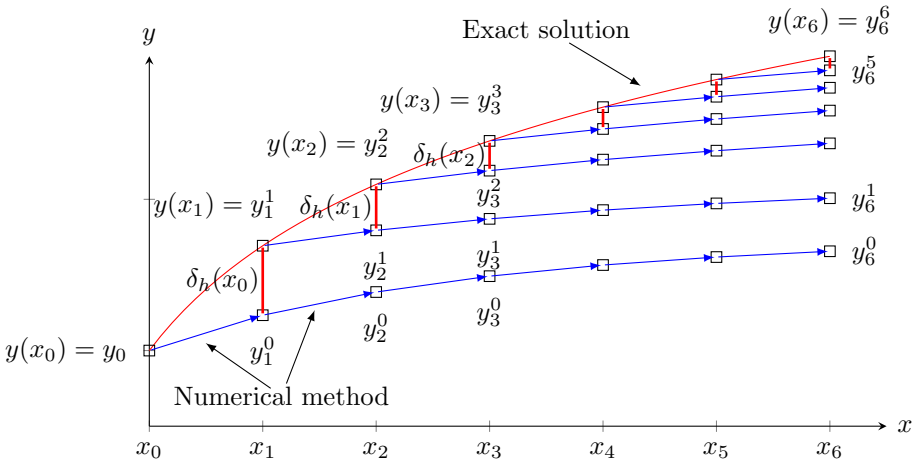


Figure 5.2: Lady Windermere's Fan

This leads to:

$$\begin{aligned}
\|\Pi_{1,n+1}\Delta q_{n+1}\| &= \|\Pi_{1,n}\Delta q_n\| + \mathcal{O}\left(h\|\Delta p_n\| + h^{m+2}\|\Delta\lambda_n\|\right)\\
\|\Pi_{2,n+1}\Delta p_{n+1}\| &= \|\Pi_{2,n}\Delta p_n\| + \mathcal{O}\left(h\|\Delta q_n\| + h^{m+2}\|\Delta\lambda_n\|\right)\\
\|\mathcal{R}_A(\infty)\Delta\lambda_{n+1}\| &= \|\mathcal{R}_A(\infty)\|^2\|\Delta\lambda_n\| + \mathcal{O}\left(\|\Delta q_n\| + \|\Delta p_n\| + h\|\Delta\lambda_n\|\right).
\end{aligned}$$

Thus, the error estimates become:

$$\begin{aligned}
\|\Delta q_n\| &\leq C_q\left(\|\Delta q_0\| + h\|\Delta p_0\| + h^{m+2}\|\Delta\lambda_0\|\right)\\
\|\Delta p_n\| &\leq C_p\left(\|\Pi_{1,0}\Delta q_0\| + \|\Pi_{2,0}\Delta p_0\| + h^{m+2}\|\Delta\lambda_0\|\right)\\
\|\Delta\lambda_n\| &\leq C_\lambda\left(\|\mathcal{R}_A(\infty)\|^n\|\Delta\lambda_0\| + \|\Delta q_0\| + \|\Delta p_0\| + h\|\Delta\lambda_0\|\right).
\end{aligned}$$

Proceeding as in [HLR89, theorem 4.4] to use the Lady Windermere's Fan construction (see fig.5.2) and using the results from theorem 5.2.6 for $\delta q_h(t_k), \delta p_h(t_k)$, and the results we derived for $\delta\lambda_h(t_k)$, with $m = \min(q-1, r, p-q, p-r)$ for $-1 \leq R(\infty) < 1$ as well as $m = \min(q-2, r, p-q, p-r)$ for $R(\infty) = 1$, we find the global error by addition of local errors, which gives the result we were looking for. □

Corollary 5.2.7.1. *The global error for the Lobatto IIIA-B method applied to the IVP posed by the partitioned differential-algebraic system of eqs.*(5.6) *is:*

$$q_n - q(t_n) = \mathcal{O}(h^{\min(2s-2)}), \tag{5.36a}$$

$$p_n - p(t_n) = \mathcal{O}(h^{\min(2s-2)}), \tag{5.36b}$$

$$\lambda_n - \lambda(t_n) = \begin{cases} \mathcal{O}(h^s) & \text{if } s \text{ even},\\ \mathcal{O}(h^{s-1}) & \text{if } s \text{ odd}. \end{cases} \tag{5.36c}$$

Proof. To prove this it suffices to substitute $p = 2s-2$, $q = s$, $r = s-2$ and $\mathcal{R}_A(\infty) = (-1)^{s-1}$ in the former theorem. □

5.3 Discrete holonomically constrained mechanical systems

We will not go into much detail here as it would take a great deal of space to delve into the details and the caveats involved in the study of holonomically constrained mechanical systems [LR04]. Conceptually and geometrically it is not a big step from the unconstrained case save for the particularities of the augmented picture, where we include Lagrange multipliers which make the augmented Lagrangian and its corresponding discrete counterpart singular. The reader is referred to [MW01; BO07; Jay96] for more information.

As in the continuous case, let $i_N : N \hookrightarrow Q$ denote the inclusion map of the submanifold N in Q. We may naturally extend this inclusion to $Q \times Q$, where discrete Lagrangians are defined, as $i_{N\times N} : N \times N \hookrightarrow Q \times Q$, $i_{N\times N}(q_0, q_1) = (i_N(q_0), i_N(q_1))$. Given a discrete Lagrangian L_d, we may define the restricted discrete Lagrangian $L_d^N = L_d \circ i_{N\times N}$.

Let us now define the augmented space, $Q \times \Lambda$, where $\Lambda \cong \mathbb{R}^m$ is the space of Lagrange multipliers and $m = \operatorname{codim}_Q N$ is the number of independent holonomic constraints. With this we may also define an augmented discrete Lagrangian $\tilde{L}_d : Q \times \Lambda \times Q \times \Lambda \to \mathbb{R}$ as an approximation to the exact discrete Lagrangian for $\tilde{L} = L + \langle \lambda, \Phi \rangle$. We will be more interested in the augmented approach, as we will use that for nonholonomic systems in the next section [see MMS15, for a more intrinsic approach using Lagrangian submanifolds]. Moreover, numerical methods are based on discretizations which have a simpler description when working on vector spaces.

Variation of the augmented discrete action leads to:

$$\begin{aligned} 0 = \delta \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) + \sum_{k=0}^{N-1} \big[\big\langle f_d^-(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}), \delta q_k \big\rangle + \\ + \big\langle f_d^+(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}), \delta q_{k+1} \big\rangle \big] + h \sum_{k=0}^{N-1} \sum_{i=1}^{s} b_i \left\langle \delta \Lambda_k^i, \Phi\left(Q_k^i\right) \right\rangle \end{aligned} \tag{5.37}$$

where:

$$f_d^-(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}) = h \sum_{i=1}^{s} b_i \left\langle \Lambda_k^i, D\Phi\left(Q_k^i\right) \frac{\partial Q_k^i}{\partial q_k}, \right\rangle \tag{5.38a}$$

$$f_d^+(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}) = h \sum_{i=1}^{s} b_i \left\langle \Lambda_k^i, D\Phi\left(Q_k^i\right) \frac{\partial Q_k^i}{\partial q_{k+1}}, \right\rangle \tag{5.38b}$$

are the forcing terms arising from the constraints. Let us assume that we discretize our Lagrangian applying the trapezoidal rule, which simplifies these to:

$$\begin{aligned} f_d^-(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}) &= \frac{h}{2} \langle \lambda_k, D\Phi(q_k) \rangle , \\ f_d^+(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}) &= \frac{h}{2} \langle \lambda_{k+1}, D\Phi(q_{k+1}) \rangle . \end{aligned}$$

Then the constrained discrete Euler-Lagrange equations take the form:

$$\begin{aligned} D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) &= -h \langle \lambda_k, D\Phi(q_k) \rangle \\ \Phi(q_k) &= 0, \quad \forall k = 0, ..., N \end{aligned}$$

which means the solution must satisfy:

$$\left(T^*i_N\right)_{q_k}\left[D_2L_d\circ i_{N\times N}(\tilde{q}_{k-1},\tilde{q}_k)+D_1L_d\circ i_{N\times N}(\tilde{q}_k,\tilde{q}_{k+1})\right]=0$$

where $\tilde{q}_k\in N$.

Using the restricted discrete Lagrangian the equations simplify to the expected:

$$D_2L_d^N(\tilde{q}_{k-1},\tilde{q}_k)+D_1L_d^N(\tilde{q}_k,\tilde{q}_{k+1})=0\,.$$

The equivalent symplectic integrator written in Hamiltonian form becomes:

$$\begin{aligned}
p_0 &= -D_1L_d(q_0,q_1)-\frac{h}{2}\left\langle\lambda_0,D\Phi(q_0)\right\rangle\\
p_1 &= D_2L_d(q_0,q_1)+\frac{h}{2}\left\langle\lambda_1,D\Phi(q_1)\right\rangle\\
0 &= \Phi(q_1)\\
0 &= \left\langle D\Phi(q_1),\frac{\partial H}{\partial p}(q_1,p_1)\right\rangle
\end{aligned}$$

where the last equation must be enforced so that $p_1\in T^*_{q_1}N$. This latter method is known as RATTLE and its augmented Lagrangian version is the SHAKE method [RCB77; And82; LS94; LR04; MW01].

Working with the augmented discrete Hamilton-Pontryagin action:

$$\begin{aligned}
\left(\widetilde{\mathcal{J}}_{\mathcal{HP}}\right)_d = \sum_{k=0}^{N-1}\sum_{i=1}^{s}hb_i\Bigg[&L\left(Q_k^i,V_k^i\right)+\left\langle\tilde{P}_k^i,\frac{Q_k^i-q_k}{h}-\sum_{j=1}^{s}a_{ij}V_k^j\right\rangle\\
&+\left\langle\tilde{p}_{k+1},\frac{q_{k+1}-q_k}{h}-\sum_{j=1}^{s}b_jV_k^j\right\rangle+\left\langle\Lambda_k^i,\Phi(Q_k^i)\right\rangle\Bigg]
\end{aligned}\tag{5.39}$$

we can obtain a constrained version of the symplectic partitioned Runge-Kutta method:

$$q_{k+1}=q_k+h\sum_{j=1}^{s}b_jV_k^j,\qquad p_{k+1}=p_k+h\sum_{j=1}^{s}\hat{b}_jW_k^j,\tag{5.40a}$$

$$Q_k^i=q_k+h\sum_{j=1}^{s}a_{ij}V_k^j,\qquad P_k^i=p_k+h\sum_{j=1}^{s}\hat{a}_{ij}W_k^j,\tag{5.40b}$$

$$W_k^i=D_1L(Q_k^i,V_k^i)+\left\langle\Lambda_k^i,D\Phi(Q_k^i)\right\rangle\quad P_k^i=D_2L(Q_k^i,V_k^i)\tag{5.40c}$$

$$0=\Phi(Q_k^i)\qquad 0=\left\langle D\Phi(q_{k+1}),D_2H(q_{k+1},p_{k+1})\right\rangle\tag{5.40d}$$

where (a_{ij},b_i) and $(\hat{a}_{ij},\hat{b}_i)$ are a pair of symplectically conjugated methods. The tangency condition on q_{k+1} (eq.(5.40d), right) must be judiciously added to close the system, allowing us to obtain a Hamiltonian map $(q_k,p_k)\mapsto(q_{k+1},p_{k+1})$.

Unfortunately, not every choice of RK method will give us the expected variational order for the Hamiltonian flow on N [see Jay93; Jay96; Jay03; MW01; JM09]. Indeed, numerical tests already tell us that a 2-stage Gauss method, whose corresponding variational order should be 4, actually has order 2 when projected to N.

Forcing the order to coincide, the corresponding augmented discrete Hamilton-Pontryagin action must restrict to N as well. To warrant that the method restricts to N we impose that (a_{ij}, b_i) satisfy the hypotheses H1, H2 and H3.

If $(\hat{a}_{ij}, \hat{b}_i)$ are the coefficients of the symplectically conjugated of the former method, then they must satisfy hypotheses H1', H2'.

Remember that H1 and H3 imply that $c_1 = 0$ and $c_s = 1$, and thus for any given $k = 0, ..., N-1$ the first and last internal stages must coincide with the nodal values, i.e. $Q_k^1 = q_k$ and $Q_k^s = q_{k+1}$, which ensures that we can impose the constraints on purely variational grounds and so the associated augmented discrete Hamilton-Pontryagin must restrict to N.

A particular member of the family is the Lobatto IIIA-B pair, whose 2-stage version is the well-known trapezoidal rule that we applied first.

5.4 Discrete nonholonomic mechanics

Naturally, we could ask ourselves whether we can construct integrators for mechanical nonholonomic systems in a similar manner as we have done with our variational integrators [Cor02; MP06; LMS04; FZ05; FIM08].

As we already discussed in section 5.1.1, nonholonomic mechanics is not variational, yet we know that Chetaev's principle is not a radical departure from Hamilton's principle and the resulting equations of motion are fairly similar to those of a holonomic system [NF72; Blo15; BM02; Cor02]. It is also true that nonholonomic mechanics is not symplectic either, so the value of applying the philosophy of symplectic integrators seems at least questionable, since there is not, in general, preservation of a symplectic or Poisson structure [SM94; Can+00]. Still, given that the departure from holonomic mechanics is not that dramatic and the structure-preserving behavior of variational integrators we still believe it is worth trying to extend our approach to nonholonomic systems.

The fact that these systems are not variational implies that the important result of theorem 3.2.2 does not apply anymore, which strips us from one of our main tools to prove the order of the resulting methods. This leaves us with standard numerical analysis techniques and results to try and prove the order on a *per family* basis. Again we will focus on symplectic RK pairs satisfying all the hypotheses stated in the holonomically constrained case.

Without further ado, we present the following *nonholonomic partitioned Runge-Kutta integrator*: Let (L, Φ) be a regular nonholonomic Lagrangian system, with $\Psi = \Phi \circ \mathbb{F}L^{-1}$, then the equations for the integrator are:

$$q_{k+1} = q_k + h \sum_{i=1}^{s} b_i V_k^i, \qquad p_{k+1} = p_k + h \sum_{i=1}^{s} \hat{b}_i W_k^i, \tag{5.41a}$$

$$Q_k^i = q_k + h \sum_{j=1}^{s} a_{ij} V_k^j, \qquad P_k^i = p_k + h \sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \tag{5.41b}$$

$$W_k^i = D_1 L(Q_k^i, V_k^i) + \left\langle \Lambda_k^i, D_2 \Phi(Q_k^i, V_k^i) \right\rangle, \quad P_k^i = D_2 L(Q_k^i, V_k^i), \tag{5.41c}$$

$$q_k^i = Q_k^i, \qquad p_k^i = p_k + h \sum_{j=1}^{s} a_{ij} W_k^j, \tag{5.41d}$$

$$\Psi(q_k^i, p_k^i) = 0 \tag{5.41e}$$

where (q_k, p_k, λ_k) are the initial data that must be supplied. This generates a flow

$$\begin{array}{rccc} \widetilde{F}_{L_d,\Lambda}: & T^*Q|_M \times \Lambda & \to & T^*Q|_M \times \Lambda \\ & (q_k, p_k, \lambda_k = \Lambda_k^1) & \mapsto & (q_{k+1}, p_{k+1}, \lambda_{k+1} = \Lambda_k^s). \end{array}$$

Of course, it is possible to apply the continuous fibre derivative $\mathbb{F}L$, and work only with Φ and forget about Ψ. We only need to introduce the variables $v_k, v_k^i \in TQ$ implicitly defined using the continuous Lagrangian by $p_k = D_2L(q_k, v_k)$ and $p_k^i = D_2L(q_k^i, v_k^i)$ respectively and change the constraint equations to $\Phi(q_k^i, v_k^i)$, thus generating the flow

$$\begin{array}{rccc} \widehat{F}_{L_d,\Lambda}: & TQ|_N \times \Lambda & \to & TQ|_N \times \Lambda \\ & (q_k, v_k, \lambda_k = \Lambda_k^1) & \mapsto & (q_{k+1}, v_{k+1}, \lambda_{k+1} = \Lambda_k^s). \end{array}$$

A purely Hamiltonian version of this method would be:

$$q_{k+1} = q_k + h\sum_{i=1}^{s} b_i V_k^i, \qquad p_{k+1} = p_k - h\sum_{i=1}^{s} \hat{b}_i W_k^i, \tag{5.42a}$$

$$Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, \qquad P_k^i = p_k - h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \tag{5.42b}$$

$$V_k^i = D_2H(Q_k^i, P_k^i), \qquad W_k^i = D_1H(Q_k^i, P_k^i) - \left\langle \Lambda_k^i, \flat_H \left(D_2\Psi\right)(Q_k^i, P_k^i)\right\rangle, \tag{5.42c}$$

$$q_k^i = Q_k^i, \qquad p_k^i = p_k - h\sum_{j=1}^{s} a_{ij} W_k^j, \tag{5.42d}$$

$$\Psi(q_k^i, p_k^i) = 0. \tag{5.42e}$$

The method admits a similar interpretation as its holonomic counterpart:

$$\begin{aligned} 0 = \delta\sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) + \sum_{k=0}^{N-1} \big[\big\langle f_{d,nh}^-(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}), \delta q_k\big\rangle + \\ + \left\langle f_{d,nh}^+(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}), \delta q_{k+1}\right\rangle\big] + h\sum_{k=0}^{N-1}\sum_{i=1}^{s} b_i \left\langle \delta\Lambda_k^i, \Phi\left(q_k^i, v_k^i\right)\right\rangle \end{aligned} \tag{5.43}$$

where now eqs.(5.38) become:

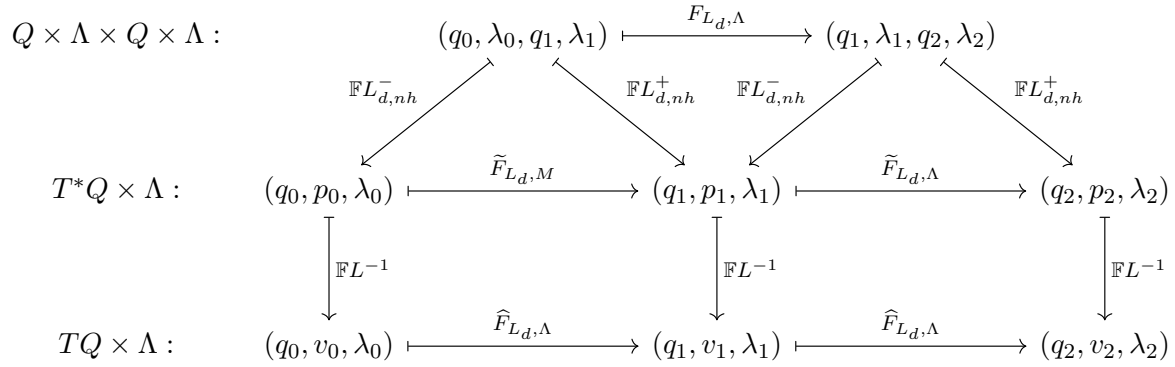
$$f_{d,nh}^-(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}) = h\sum_{i=1}^{s} b_i \left\langle \Lambda_k^i, D_2\Phi\left(Q_k^i, V_k^i\right)\frac{\partial Q_k^i}{\partial q_k}\right\rangle \tag{5.44a}$$

$$f_{d,nh}^+(q_k, \lambda_k, q_{k+1}, \lambda_{k+1}) = h\sum_{i=1}^{s} b_i \left\langle \Lambda_k^i, D_2\Phi\left(Q_k^i, V_k^i\right)\frac{\partial Q_k^i}{\partial q_{k+1}}\right\rangle \tag{5.44b}$$

with $\lambda_k = \Lambda_k^1$ and $\lambda_{k+1} = \Lambda_k^s$. Note that once q_k, λ_k and q_{k+1} are set, λ_{k+1} is fixed by the equations of the integrator. Still, these allow us to define discrete nonholonomic Legendre transformations *over the solutions of the integrator*:

$$\begin{aligned}\mathbb{F}L^-_{d,nh}(q_0,\lambda_0,q_1,\lambda_1) &= (q_0, p_0 = -D_1L_d(q_0,q_1) - f^-_{d,nh}(q_k,\lambda_k,q_{k+1},\lambda_{k+1}),\lambda_0)\\ \mathbb{F}L^+_{d,nh}(q_0,\lambda_0,q_1,\lambda_1) &= (q_1, p_1 = D_2L_d(q_0,q_1) + f^+_{d,nh}(q_k,\lambda_k,q_{k+1},\lambda_{k+1}),\lambda_1)\,.\end{aligned}$$

Thus, formally we can write the scheme of our integrator as



where $F_{L_d,\Lambda}$ is implicitly defined to close the diagram.

Theorems 5.2.6 and 5.2.7 can be used to show that the order of this method coincides with its holonomic equivalent for Lobatto-type methods. In particular, from corollary 5.2.7.1, we get that the global error for the Lobatto IIIA-B method applied to eqs.(5.41) is:

$$q_N - q(t_N) = \mathcal{O}(h^{\min(2s-2)}) \tag{5.45a}$$

$$p_N - p(t_N) = \mathcal{O}(h^{\min(2s-2)}) \tag{5.45b}$$

$$\lambda_N - \lambda(t_N) = \begin{cases} \mathcal{O}(h^s) & \text{if } s \text{ even},\\ \mathcal{O}(h^{s-1}) & \text{if } s \text{ odd}.\end{cases} \tag{5.45c}$$

Proof. To prove this, it suffices to substitute $p = 2s-2$, $q = s$, $r = s-2$ and $\mathcal{R}_A(\infty) = (-1)^{s-1}$ in the former theorem. □

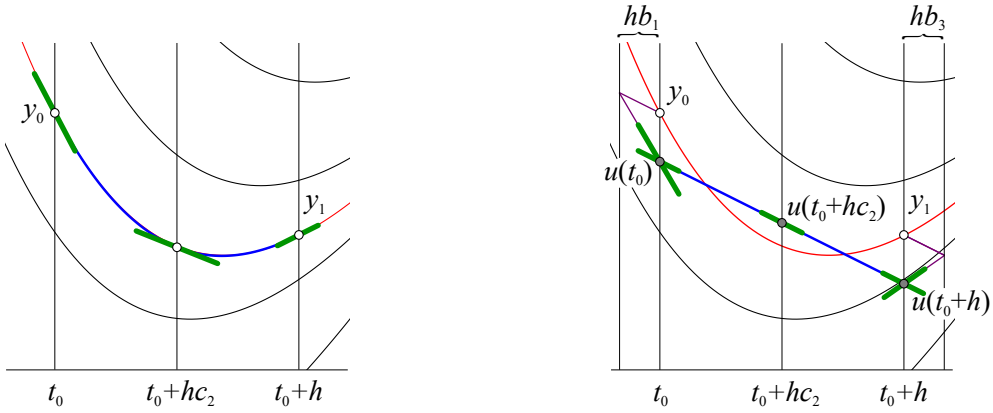
These prove that the order of our method on the submanifold M corresponds to the expected order.

5.4.1 Origin and idea behind the algorithm

What would the nonholonomic SHAKE look like? Let us look back at the holonomic case and in particular at eq.(5.37). We see that we need to determine an adequate forcing and impose the constraints.

The natural way to extend the forcing found in the holonomic case, eqs.(5.38), would be as was already shown in eqs.(5.44). If we apply the trapezoidal rule, these simplify to:

$$\begin{aligned}f_d^-(q_k,q_{k+1},\lambda_k,\lambda_{k+1}) &= \frac{h}{2}\left\langle \lambda_k, D_2\Phi\left(q_k, \frac{q_{k+1}-q_k}{h}\right)\right\rangle,\\ f_d^+(q_k,q_{k+1},\lambda_k,\lambda_{k+1}) &= \frac{h}{2}\left\langle \lambda_{k+1}, D_2\Phi\left(q_{k+1}, \frac{q_{k+1}-q_k}{h}\right)\right\rangle.\end{aligned}$$



(a) Continuous collocation

(b) Discontinuous collocation

Figure 5.3: On the left we have a continuous collocation method where the collocation polynomial (in blue) tries to give a good continuous approximation of the solution (in red). On the right we have a discontinuous collocation method applied to the same problem. The collocation polynomial $u(t)$ is a poor approximation of the solution, particularly at collocation points, but it allows us to compute y_1 to the same order as the continuous method.

As for the constraint, we could enforce $\Phi(Q_k^i, V_k^i) = 0$, which in the trapezoidal case would lead to:

$$\Phi\left(q_k, \frac{q_{k+1}-q_k}{h}\right) = \Phi\left(q_{k+1}, \frac{q_{k+1}-q_k}{h}\right) = 0, \quad \forall k\,.$$

Note that this would not warrant that our integrator would preserve the continuous constraint, $\Phi(q_k, v_k) = \Phi(q_{k+1}, v_{k+1}) = 0$, where $v_k = \mathbb{F}L^{-1}(p_k)$. Also, this is a direct discretization of the constraint manifold, which feels both arbitrary and rough. The more sensible option is indeed to impose the preservation of the continuous constraint, which we prefer to impose as $\Psi(q_k, p_k) = \Psi(q_{k+1}, p_{k+1}) = 0$. Thus, the integrator becomes:

$$D_2L_d(q_{k-1}, q_k) + D_1L_d(q_k, q_{k+1}) = -h\left\langle \lambda_k, D_2\Phi\left(q_k, \frac{q_{k+1}-q_k}{h}\right)\right\rangle$$
$$\Psi(q_k, p_k) = 0, \quad \forall k = 0, ..., N\,.$$

The discrete Euler-Lagrange equations are still a matching of momenta,

$$p_k^-(q_{k-1}, q_k, \lambda_k) = p_k^+(q_k, q_{k+1}, \lambda_k)$$

and we can chose either p_k^- or p_k^+ to impose the constraint without difference [see LMS04].

The question now is, how does this method generalize to higher order? When we use the Lobatto IIIA method in eqs.(3.12) and apply the discrete Hamilton-Pontryagin principle we automatically obtain the Lobatto IIIB method in eqs.(3.13) for the P_k^i momenta. The first method is a continuous collocation method (fig. 5.3a) and the second is a discontinuous collocation method (fig. 5.3b).

Continuous collocation provides a relatively good (cf. eq.(2.13)) continuous approximation of the solution whereas discontinuous (cf. eq.(2.14)) offers a poorer one, forming something akin to a scaffolding to obtain the actual nodal values p_k instead of trying to provide a good approximation on the interval (fig. 5.3). For more information on the matter, please refer to section 2.3.1.

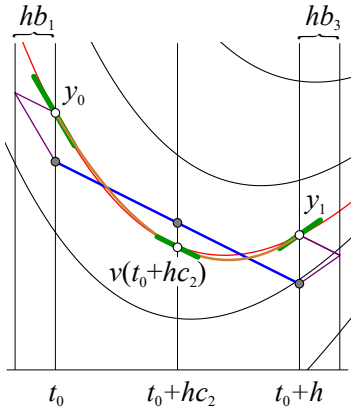


Figure 5.4: Continuous collocation polynomial $v(t)$ (in orange) obtained from discontinuous collocation data.

From the study of order conditions we know that at inner stages the convergence is related to the $C(q)$ simplifying assumption that each method satisfies, which are $C(s)$ and $\widehat{C}(s-2)$, thus coinciding in this case with the former estimates. At nodal points, the convergence is related to the $B(p)$ simplifying assumption (*superconvergence*), which both satisfy for $p = 2s-2$.

This means that, in our case, Q_k^i is an approximation of order s to $q(t_k^i)$, whereas P_k^i is an approximation of order $s-2$ to $p(t_k^i)$. If we try to enforce a nonholonomic constraint using these values we will be asking our solution to lie far away from the corresponding point that the real trajectory would pass through. Thus, the question would be whether we can generate better approximations of $p(t_k^i)$ and whether we can do this cheaply. As it turns out, we can. We only need to apply the same Lobatto IIIA quadrature rule to the momenta and, better yet, we can reuse the W_k^i values used for the determination of P_k^i. As a side effect, this provides us with a better continuous approximation of p (order $s-1$, cf. proposition 5.4.1), although not as good as the continuous approximation of q (see fig.5.4).

Surprisingly, the new values we obtain using this method, which we call p_k^i, are an approximation of order s to our desired $p(t_k^i)$. This is so because the Lobatto IIIA-B pair satisfies the mixed simplifying assumption $C\widehat{C}(s)$ [Jay96].

Intuitively speaking, enforcing the constraints with these should give better results. These better estimates of $p(t_k^i)$ can be obtained for any other symplectic integrator in holonomic systems, but there they become completely decoupled and can be obtained *a posteriori*.

Proposition 5.4.1. *Let (a_{ij}, b_j) and $(\hat{a}_{ij}, \hat{b}_j)$ be the coefficients of the Lobatto IIIA-B pair. Let us solve (2.12), with f Lipschitz, and denote the resulting interpolation polynomial by $u(t)$. Then for sufficiently small h the polynomial:*

$$v(t) = y_0 + h\sum_{j=1}^{s} f(t_0 + c_j h, u(t_0 + c_j h)) \int_{t_0}^{t} \ell_j(\tau)\mathrm{d}\tau$$

is an approximation of order $s-1$ of the solution $y(t)$ in the interval $t \in [t_0, t_0+h]$, i.e.:

$$\|v(t) - y(t)\| \leq Ch^s \quad \forall t \in [t_0, t_0+h]\,.$$

Moreover, the derivatives of $u(t)$ satisfy:

$$\left\|v^{(k)}(t) - y^{(k)}(t)\right\| \leq Ch^{s-k} \quad \forall t \in [t_0, t_0+h]$$

Proof. Following [HLW10, Lemma 1.6], and using the same notation, we may express the exact solution as:

$$\dot{y}(t_0 + \tau h) = y_0 + h \sum_{j=1}^{s} f(t_0 + c_j h, y(t_0 + c_j h))\ell_j(\tau) + h^s E(\tau, h),$$

where the interpolation $E(\tau, h)$ is bound by a constant M.

By integration of the difference $\dot{y}(t_0 + \tau h) - \dot{v}(t_0 + \tau h)$ we obtain:

$$y(t_0 + \tau h) - v(t_0 + \tau h) = h \sum_{j=1}^{s} \delta f_j \int_0^\tau \ell_j(\sigma)\mathrm{d}\sigma + h^{s+1} \int_0^\tau E(\sigma, h)\mathrm{d}\sigma \tag{5.46}$$

where $\delta f_j = f(t_0 + c_j h, y(t_0 + c_j h)) - f(t_0 + c_j h, u(t_0 + c_j h))$.

Now, invoking the result of [HLW10, Lemma 1.10]:

$$\|u(t) - y(t)\| \leq Ch^{s-1} \quad \forall t \in [t_0, t_0 + h]$$

we finally get that:

$$\|y(t) - v(t)\| \leq hC \|y(t) - u(t)\| + h^{s+1}M \leq CLh^s + h^{s+1}M\,.$$

Derivation of (5.46) and further application of the same lemma proves the second statement. □

5.4.2 Hamilton-Jacobi point of view of the integrator

We are trying to generate a numerical integrator of a known order in $N \subset TQ$. Contrary to the holonomically constrained case, the inclusion map $i_N : N \hookrightarrow TQ$ does not naturally induce a submanifold in $Q \times Q$, so we cannot generate a discrete constrained Lagrangian as we could in that case.

First, consider the nonholonomic Lagrangian system

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\left(\dfrac{\partial L}{\partial \dot{q}^i}\right) - \dfrac{\partial L}{\partial q^i} = \left\langle \lambda, \dfrac{\partial \Phi}{\partial \dot{q}^i} \right\rangle, \\ \Phi(q, \dot{q}) = 0. \end{cases}$$

In principle nonholonomic mechanics is only defined on N, but we may extend the dynamical vector field to all of TQ by simply removing the constraint equations. In that case the Lagrange multipliers are completely free and undetermined.

Provided the Lagrangian is regular, we may write this set of equations as

$$\ddot{q}^i(t) = F^i(q, \dot{q}, \lambda),$$

or, better yet, as the first order system

$$\begin{cases} \dot{q}^i(t) = v^i\,, \\ \dot{v}^i(t) = F^i(q, v, \lambda)\,. \end{cases} \tag{5.47}$$

This defines a vector field $X_L : TQ \times \Lambda \to TTQ$.

In order for this system to produce the same dynamics as the original nonholonomic system we must consider the constraint equations. If the compatibility conditions with

the constraint are met, then we can find explicit expressions for the Lagrange multipliers using the condition

$$\imath_{X_L}\Phi = 0,$$

that is, by differentiating the constraint and inserting the resulting expression in the first order system above. This way we obtain $\lambda_\alpha = \kappa_\alpha(q, v)$. Note that with this we may also construct an augmented inclusion map $\hat{\imath}_{N,\Lambda} : N \to TQ \times \Lambda$.

It should also be noted that the resulting expression for λ_α remains the same if we allow for Φ to take any value, not just 0. Once an initial condition $(q_0, v_0) \in TQ$ is set, if we insert $\kappa_\alpha(q, v)$ in eqs. (5.47), the evolution of the system will be such that $\Phi(q, v) = \Phi(q_0, v_0) = \text{const}$. This is tantamount to a redefinition of the constraint equations, $\Phi' = \Phi - \Phi(q_0, v_0)$, and therefore a new constraint submanifold $N' \subset TQ$.

Moreover, by differentiating the constraint equations we can construct a new differential system

$$\begin{cases} \dot{q}^i(t) = v^i\,, \\ \dot{v}^i(t) = F^i(q, v, \lambda)\,, \\ \dot{\lambda}_\alpha(t) = K_\alpha(q, v, \lambda)\,, \end{cases} \tag{5.48}$$

where

$$K_\alpha(q, v, \lambda) = \frac{\partial \kappa_\alpha}{\partial q^i} v^i + \frac{\partial \kappa_\alpha}{\partial v^i} F^i(q, v, \lambda)\,.$$

This new system defines a vector field in $X_{L,\Lambda} \in \mathfrak{X}(TQ \times \Lambda)$ with flow $F^{\Delta t}_{L,\Lambda} : TQ \times \Lambda \to TQ \times \Lambda$. This flow should be well defined, at least for a small enough Δt. Clearly, if initial values $(q_0, v_0, \kappa(q_0, v_0))$ are chosen for this system so that $\Phi(q, v) = 0$, then the flow of this vector field projects onto the flow of the original nonholonomic system.

As the Lagrangian is assumed to be regular we can use the fibre derivative to define an associated Hamiltonian $H : T^*Q \to \mathbb{R}$, constraint function $\Psi : T^*Q \to \mathbb{R}^m$ and constraint submanifold $M \subset T^*Q$ (see section 5.1.2). Similarly, we can define new functions $\tilde{\kappa}_\alpha = \kappa_\alpha \circ (\mathbb{F}L)^{-1}$, $\alpha = 1, ..., m$. The null-set of Ψ together with $\tilde{\kappa}$ induce an augmented inclusion map $\tilde{\imath}_{M,\Lambda} : M \to T^*Q \times \Lambda$.

We can also generate an equivalent system to that in eq.(5.48) on the Hamiltonian side:

$$\begin{cases} \dot{q}^i(t) = \dfrac{\partial H}{\partial p_i}\,, \\ \dot{v}^i(t) = -\dfrac{\partial H}{\partial q^i} + \left\langle \lambda, (g_H)_{ij} \dfrac{\partial \Psi}{\partial p_j} \right\rangle\,, \\ \dot{\lambda}_\alpha(t) = \widetilde{K}_\alpha(q, p, \lambda)\,, \end{cases}$$

where now

$$\widetilde{K}_\alpha(q, p, \lambda) = \frac{\partial \tilde{\kappa}_\alpha}{\partial q^i} \frac{\partial H}{\partial p_i} - \frac{\partial \tilde{\kappa}_\alpha}{\partial p_i} \left(\frac{\partial H}{\partial q^i} - \left\langle \lambda, (g_H)_{ij} \frac{\partial \Psi}{\partial p_j} \right\rangle \right)\,.$$

Therefore, we may also build a flow $\widetilde{F}^{\Delta t}_{L,\Lambda} : T^*Q \times \Lambda \to T^*Q \times \Lambda$.

An exact discrete Lagrangian for the nonholonomic problem should be defined as a complete solution of the corresponding nonholonomic Hamilton-Jacobi equation [ILM08; OB09]. Let us assume that the constraints are linear so that conservation of energy is guaranteed, and we need not move on to the time-dependent setting.

In contrast with the holonomic case, in general the nonholonomic Hamilton-Jacobi equation is not an equation for a function $S : Q \times Q \to \mathbb{R}$ but for a 1-form $\Gamma : Q \times Q \to$

$T^*Q|_M \times T^*Q|_M$. If by Γ_{q_0} and Γ_{q_1} we denote the projections of Γ onto its first and second component, then it must satisfy the system

$$\begin{aligned} H\left(q_0, -\Gamma_{q_0}(q_0, q_1)\right) &= E \\ H\left(q_1, \Gamma_{q_1}(q_0, q_1)\right) &= E \end{aligned}$$

with $E = \text{const}$. We will disregard all considerations of existence and uniqueness for this Γ, and work formally.

In the augmented setting, that is, including the Lagrange multipliers as independent variables, we might have something of the form $\Gamma^\Lambda : Q \times \Lambda \times Q \to \bigwedge^1(Q \times Q)$ satisfying:

$$\begin{aligned} H\left(q_0, -\Gamma^\Lambda_{q_0}(q_0, \lambda_0, q_1)\right) &= E \\ H\left(q_1, \Gamma^\Lambda_{q_1}(q_0, \lambda_0, q_1)\right) &= -E \\ \Psi\left(q_0, -\Gamma^\Lambda_{q_0}(q_0, \lambda_0, q_1)\right) &= 0\,. \end{aligned}$$

Then, according to the framework for forced systems, we could write Γ^Λ explicitly as:

$$\begin{aligned} \Gamma^\Lambda(q_0, \lambda_0, q_1) &= \left(\frac{\partial S}{\partial q_0}(q_0, q_1) - T_{q_0}(q_0, \lambda_0, q_1)\right) \mathrm{d}q_0 \\ &= \left(\frac{\partial S}{\partial q_1}(q_0, q_1) - T_{q_1}(q_0, \lambda_0, q_1)\right) \mathrm{d}q_1. \end{aligned}$$

In this expression, S is of the same form as eq.(3.8) with $c = (q(t)) \in \tilde{C}^2(q_0, q_1, [t_0, t_1])$, satisfying Chetaev's principle and T_i are defined in terms of the constraint force as

$$\begin{aligned} T_{q_0} &= \int_{t_0}^{t_1} \left\langle \Lambda_L(\hat{c}_\lambda(t)), \frac{\partial c(t)}{\partial q_0} \right\rangle \mathrm{d}t, \\ T_{q_1} &= \int_{t_0}^{t_1} \left\langle \Lambda_L(\hat{c}_\lambda(t)), \frac{\partial c(t)}{\partial q_1} \right\rangle \mathrm{d}t. \end{aligned}$$

Here $c_\lambda(t) = (q(t), \lambda(t)) \in Q \times \Lambda$ is the augmented solution of the problem such that it projects on c (with $c_\lambda(t_0) = (q_0, \lambda_0)$) and $\hat{c}_\lambda(t) = (q(t), \dot{q}(t), \lambda(t)) \in TQ \times \Lambda$ is its tangent lift. We may write Λ_L, the Chetaev forcing form of the system, as:

$$\Lambda_L(q, v, \lambda) = \left\langle \lambda, \frac{\partial \Phi}{\partial v^i}(q, v) \right\rangle \mathrm{d}q^i\,.$$

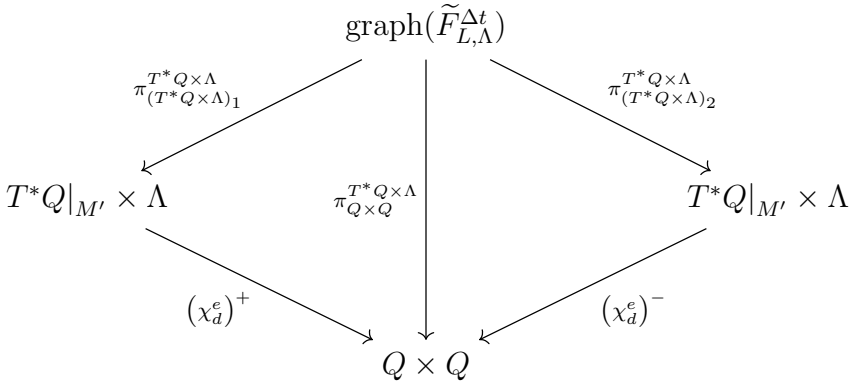
It is possible to extend these definitions to any curve $c_\lambda(t)$ satisfying eq.(5.48) instead of those satisfying the original nonholonomic system. In that case they will not be solutions of the nonholonomic Hamilton-Jacobi equation as written above, but a modified one with $\Psi\left(q_0, -\Gamma^\Lambda_{q_0}(q_0, \lambda_0, q_1)\right) = \text{const}$. Therefore, these solutions will be $\Gamma : Q \times Q \to T^*Q|_{M'} \times T^*Q|_{M'}$, with some $M' \subset T^*Q$ generally different from M but diffeomorphic to it.

Given a Γ^Λ, let us define the functions $\left(\Gamma^{\Lambda,e}_d\right)^\pm : Q \times \Lambda \times Q \to T^*Q \times \Lambda$ by:

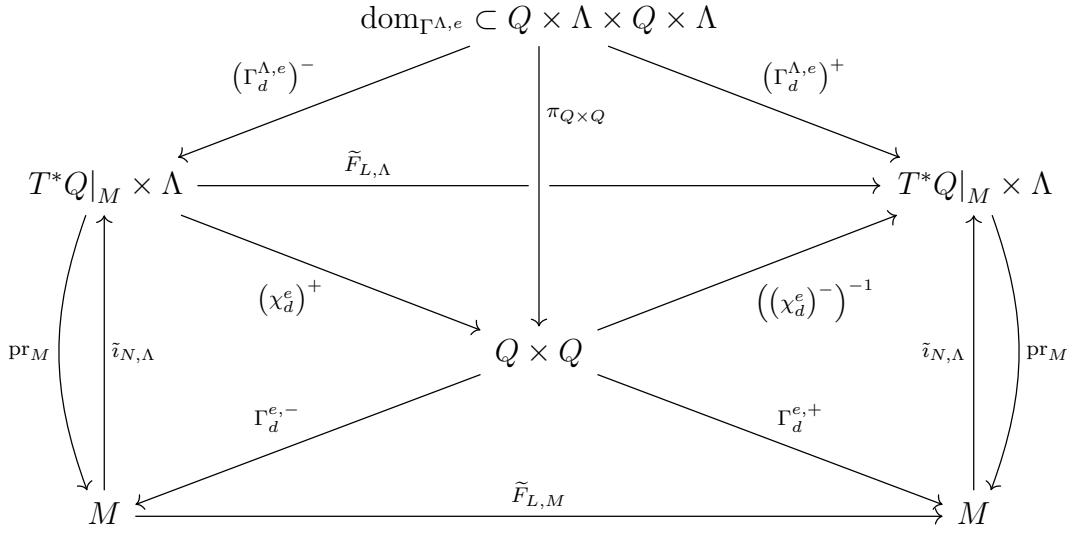
$$\begin{aligned} \left(\Gamma^{\Lambda,e}_d\right)^- &: (q_0, \lambda_0, q_1) \mapsto \left(q_0, -\Gamma^\Lambda_{q_0}(q_0, \lambda_0, q_1), \lambda_0\right) \\ \left(\Gamma^{\Lambda,e}_d\right)^+ &: (q_0, \lambda_0, q_1) \mapsto \left(q_1, \Gamma^\Lambda_{q_1}(q_0, \lambda_0, q_1), \kappa(q_1, \Gamma^\Lambda_{q_1}(q_0, \lambda_0, q_1))\right) \end{aligned}$$

which play the role of the exact discrete fibre derivatives in the forced and in the holonomic case. These are precisely the functions that the integrator is approximating.

Note that $\operatorname{graph}(\widetilde{F}_{L,\Lambda}^{\Delta t}) \subset T^*Q \times \Lambda \times T^*Q \times \Lambda$. If $\dim Q = n$, $\dim N = \dim M = 2n - m$, and $\dim \Lambda = m$, then $\dim \operatorname{graph}(\widetilde{F}_{L,\Lambda}^{\Delta t}) = \dim M + \dim \Lambda = 2n$. If we define the projectors $\pi_{Q\times Q}^{T^*Q\times\Lambda} : T^*Q \times \Lambda \times T^*Q \times \Lambda \to Q \times Q$, $\pi_{(T^*Q\times\Lambda)_{1,2}}^{T^*Q\times\Lambda} : T^*Q \times \Lambda \times T^*Q \times \Lambda \to T^*Q \times \Lambda$, then it should be possible to show that there exist two local diffeomorphisms, $(\chi_d^e)^{\pm} : T^*Q|_M \times \Lambda \to Q \times Q$, defined so that the following diagram commutes:

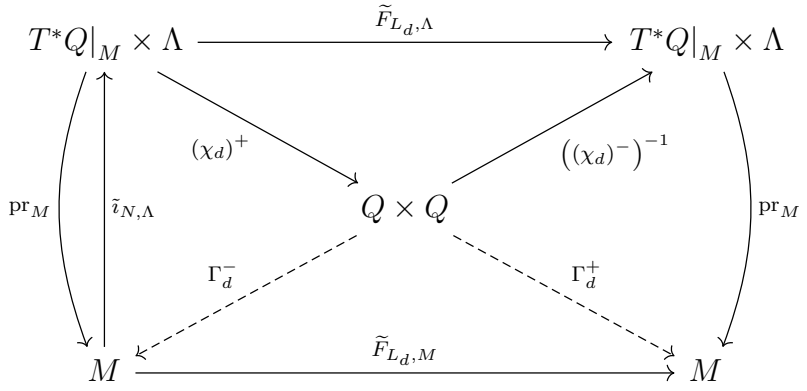


This way, if Γ^Λ is a complete solution of the nonholonomic Hamilton-Jacobi equation, the following diagram commutes:



where pr_M is just the projection of an element of $T^*Q|_M$ to M itself and $\widetilde{F}_{L,M} = \operatorname{pr}_M \circ \widetilde{F}_{L,\Lambda} \circ \tilde{\imath}_{M,\Lambda}$ is the flow on the constraint manifold. Also, $\Gamma_d^{e,\pm} : Q \times Q \to M$ are defined so that the diagram commutes. In principle, if an exact discrete constrained Lagrangian could be found, ideally these should be its associated fibre derivatives.

Our integrator provides then an approximation of $\widetilde{F}_{L,\Lambda}^h$, which we shall call $\widetilde{F}_{L_d,\Lambda}$ (the induced discrete flow), and approximations of $\left(\Gamma_d^{\Lambda,e}\right)^{\pm}$ and $(\chi_d^e)^{\pm}$, $\left(\Gamma_d^{\Lambda}\right)^{\pm}$ and $(\chi_d)^{\pm}$ respectively. The restriction of our integrator to M after a choice of λ_0 has been made (in this case, it is just $\tilde{\kappa}(q_0, p_0)$) can be represented by the flow $\widetilde{F}_{L_d,M}^{\lambda_0} = \operatorname{pr}_M \circ \widetilde{F}_{L_d,\Lambda} \circ \tilde{\imath}_{M,\Lambda}$. As it turns out, in general $\tilde{\imath}_{M,\Lambda} \circ \widetilde{F}_{L_d,M}^{\lambda_0} \circ \operatorname{pr}_M \neq \widetilde{F}_{L_d,M}$, i.e. the value of λ_1 approximated by our integrator does not coincide with the value one would obtain by applying $\tilde{\kappa}(q_1, p_1)$. Therefore, the scheme of our integrator is



This failure to close leads to the necessity of choosing a way to continue the integration process. Either we feed the integrator the λ_{k+1} obtained from (q_k, p_k, λ_k) via our integration scheme, or compute λ_{k+1} from (q_{k+1}, p_{k+1}). We choose the first method, as it seems to display the best results in terms of energy (quasi-)conservation.

5.5 Lie group integrators

For an introduction to these methods, please check section 3.4.

5.5.1 Holonomic constraints

In order to consider nonholonomic constraints we will first check the holonomic case. Assume now that our system is subjected to a set of holonomic constraints locally spanned by a function $\Phi : G \to \mathbb{R}^m$. The inclusion of these constraints amounts to the addition of a new set of terms to the discrete Hamilton-Pontryagin action, eq.(3.23):

$$\left(\widetilde{\mathcal{J}}_{\mathcal{HP}}\right)_d = \left(\mathcal{J}_{\mathcal{HP}}\right)_d + \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \Lambda_k^i, \Phi(g_k\tau(\Xi_k^i))\right\rangle .$$

Once more, we restrict to methods satisfying hypotheses H1, H2 and H3. Variation of these new terms produces the following:

$$\begin{aligned}
\delta g: \quad & \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \Lambda_k^i, \left\langle D\Phi(g_k\tau(\Xi_k^i)), \delta g_k\tau(\Xi_k^i)\right\rangle\right\rangle \\
& = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \left\langle \Lambda_k^i, \left(\mathrm{d}^L\tau^{-1}_{-\Xi_k^i}\right)^* \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{g_k\tau(\Xi_k^i)} D\Phi(g_k\tau(\Xi_k^i))\right\rangle, \zeta_k\right\rangle , \\
\delta\Xi: \quad & \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \Lambda_k^i, \left\langle D\Phi(g_k\tau(\Xi_k^i)), g_k D\tau(\Xi_k^i)\delta\Xi_k^i\right\rangle\right\rangle \\
& = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \left\langle \Lambda_k^i, \left(\mathrm{d}^L\tau_{\Xi_k^i}\right)^* L^*_{g_k\tau(\Xi_k^i)} D\Phi(g_k\tau(\Xi_k^i))\right\rangle, \delta\Xi_k^i\right\rangle , \\
\delta\Lambda: \quad & \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left\langle \delta\Lambda_k^i, \Phi(g_k\tau(\Xi_k^i))\right\rangle .
\end{aligned}$$

The first two manifest in a modification of eqs.(3.26) and (3.27) with $\mathrm{N}_k^i \mapsto \mathrm{N}_k^i + \mathrm{T}_k^i$, where:

$$\mathrm{T}_k^i = \left\langle \Lambda_k^i, \left(\mathrm{d}^L \tau_{\Xi_k^i}\right)^* L^*_{g_k\tau(\Xi_k^i)} D\Phi(g_k\tau(\Xi_k^i)) \right\rangle.$$

Of course, the variations in Λ are nothing more than the constraint equations themselves, which must be added to the rest of the equations.

As in the vector space case, we will still need to add the tangency condition to these equations to generate a well-defined Hamiltonian map $\tilde{\mathcal{F}}_{L_d} : (g_k, \mu_k) \mapsto (g_{k+1}, \mu_{k+1})$. This final equation must read:

$$\left\langle L^*_{g_{k+1}} D\Phi(g_{k+1}), D_2\hbar\left(g_{k+1}, \mu_{k+1}\right) \right\rangle = 0$$

where $\hbar : G \times \mathfrak{g}^* \to \mathbb{R}$ is the corresponding reduced Hamiltonian function.

5.5.2 Nonholonomic constraints

This time, assume that our system is subjected to a set of nonholonomic constraints locally spanned by a function $\Phi : TG \to \mathbb{R}^m$ and that $\Phi \circ \mathbb{F}L^{-1} = \Psi : T^*G \to \mathbb{R}^m$.

Applying the same reasoning as in the vector space case, it is clear that we need to apply the substitution $\mathrm{N}_k^i \mapsto \mathrm{N}_k^i + (\mathrm{T}_{\mathrm{nh}})_k^i$, where:

$$(\mathrm{T}_{\mathrm{nh}})_k^i = \left\langle \Lambda_k^i, \left(\mathrm{d}^L \tau_{\Xi_k^i}\right)^* L^*_{g_k\tau(\Xi_k^i)} D_2\Phi\left(g_k\tau(\Xi_k^i), g_k\tau(\Xi_k^i)\mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right) \right\rangle.$$

Aside from that, we need to introduce the equations

$$\mu_k^i = \mathrm{Ad}^*_{\tau(\Xi_k^i)} \left[\mu_k + h \sum_{j=1}^{s} a_{ij} \left(\mathrm{d}^L \tau^{-1}_{-\Xi_k^j}\right)^* \mathrm{N}_k^j \right],$$

together with the constraint equations

$$\Psi\left(g_k\tau(\Xi_k^i), L^*_{\left(g_k\tau(\Xi_k^i)\right)^{-1}} \mu_k^i\right) = 0.$$

If the constraint functions can be (left) trivialized so that we can write $\phi : G \times \mathfrak{g} \to \mathbb{R}^m$ and $\psi : G \times \mathfrak{g}^* \to \mathbb{R}^m$, then

$$(\mathrm{T}_{\mathrm{nh}})_k^i = \left\langle \Lambda_k^i, \left(\mathrm{d}^L \tau_{\Xi_k^i}\right)^* D_2\phi\left(g_k\tau(\Xi_k^i), \mathrm{d}^L\tau_{\Xi_k^i}\mathrm{H}_k^i\right) \right\rangle,$$

and the constraint equations that must be imposed become

$$\psi\left(g_k\tau(\Xi_k^i), \mu_k^i\right) = 0.$$

For the resulting nonholonomic integrators the results of theorems 5.2.6 and 5.2.7 still hold thanks to the way in which we have handled the discretisation. Thus, the order of these integrators matches the expected order one would obtain in the holonomic case.

5.6 Numerical tests

In this section we study several nonholonomic systems using our methods. These will allow us to compare our theoretical results with actual numerical simulations and show some of the properties of our integrators.

5.6.1 Nonholonomic particle in a harmonic potential

In this case we have $Q = \mathbb{R}^3$ and its corresponding Lagrangian and constraint functions can be written as

$$L(x, y, z, v_x, v_y, v_z) = \frac{1}{2}(v_x^2 + v_y^2 + v_z^2) - \frac{1}{2}(x^2 + y^2),$$
$$\Phi(x, y, z, v_x, v_y, v_z) = v_z - y v_x.$$

This is a classic nonholonomic system frequently used as an academic example. As it can be seen in fig. 5.5, the numerical order obtained coincides with the expected one.

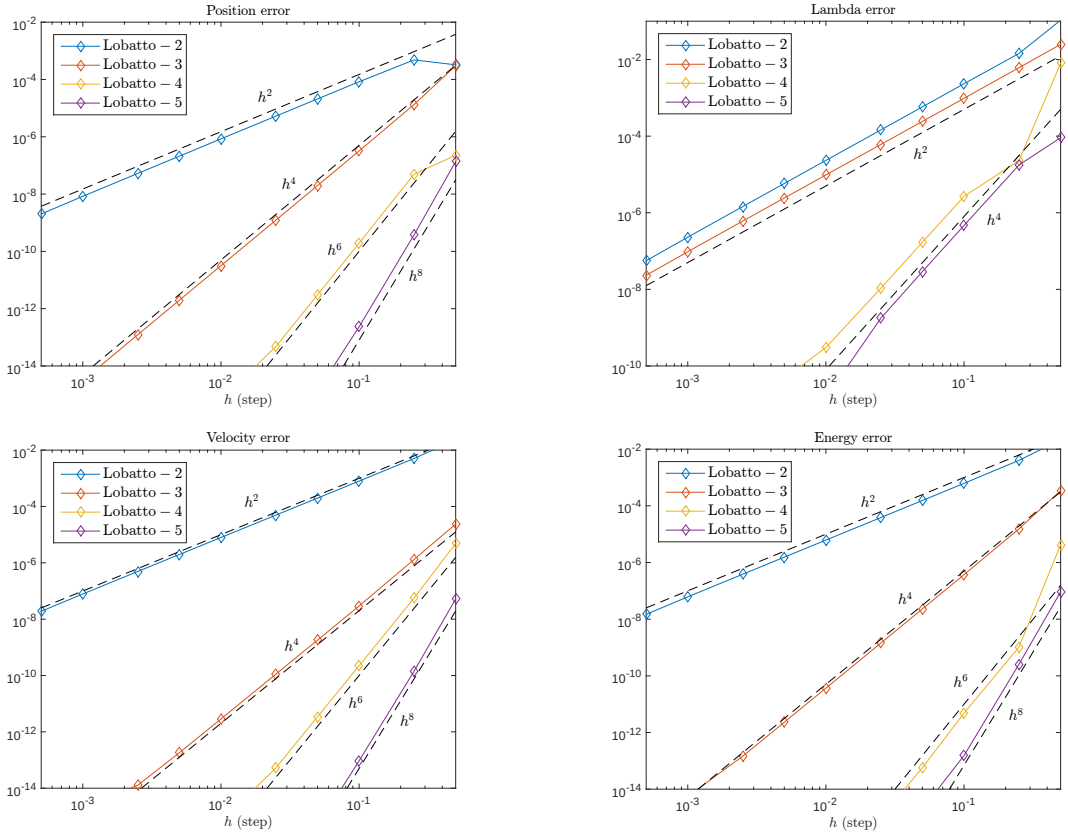


Figure 5.5: Relative error w.r.t. reference values obtained for $h =$ `1e-4` for integrators of various orders. As can be seen, the behavior of the Lagrange multipliers differs from the other variables, as predicted.

5.6.2 Pendulum-driven continuous variable transmission (CVT)

For the sake of simplicity let us consider $Q = \mathbb{R}^3$ as the configuration manifold for this system. Its corresponding Lagrangian and constraint functions are

$$L(x, y, z, v_x, v_y, v_z) = \frac{1}{2}(v_x^2 + v_y^2 + v_z^2) - \frac{1}{2}\left(x^2 + z^2 - 2\cos(y) + \epsilon \sin(2y)\right),$$
$$\Phi(x, y, z, v_x, v_y, v_z) = v_z + \sin(y) v_x$$

with $\epsilon \geq 0$. This system was featured in a recent preprint, [MV14], where it was used as a benchmark for the behavior of different numerical integrators. In particular, those authors wanted to draw attention to the behavior of the energy of the (x, z, v_x, v_z), *passenger*, and

(y, v_y), *driver*, subsystems when $\epsilon = 0, \frac{1}{2}$. This is done for two sets of initial conditions, one corresponding to low energy where the driver subsystem is restricted to its oscillatory regime, and one corresponding to high energy where the driver subsystem rotates.

The corresponding initial conditions are

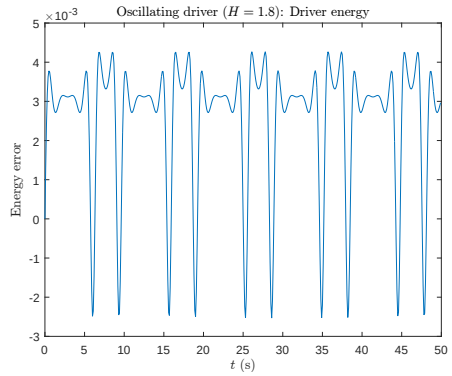
$$\vec{\mathbf{q}}_0 = (1, 0, 1)\,, \quad \vec{\mathbf{v}}_0 = \left(0, \frac{3\sqrt{10}}{5}, 0\right)$$

for the low energy case, with total energy $E_T = \frac{9}{5}$ ($E_d = \frac{4}{5}$, $E_p = 1$), and

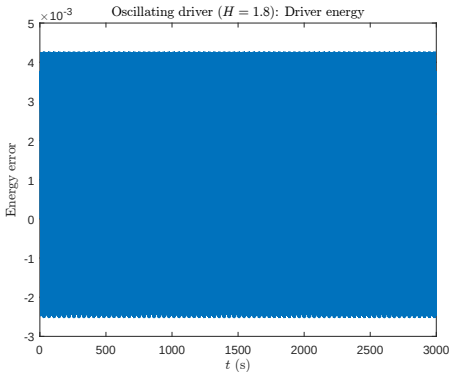
$$\vec{\mathbf{q}}_0 = (1, 0, 1)\,, \quad \vec{\mathbf{v}}_0 = \left(0, \sqrt{8}, 0\right)$$

for the high energy case, with total $E_T = 4$ ($E_d = 3$, $E_p = 1$).

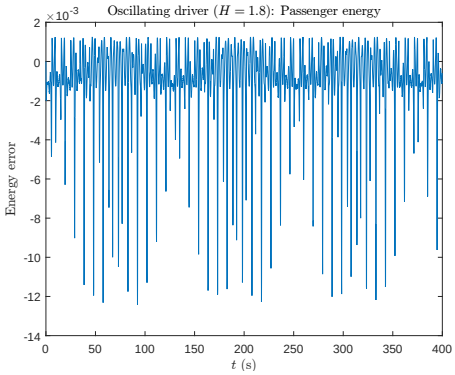
It is interesting to note that for the time step chosen in that paper, namely $h = \pi/10$, our integrator exhibits rather erratic behavior which suggests that the step might be too big. If a more sensible value, such as $h = 1/10$ is chosen, our integrator displays excellent energy behavior, as can be seen in figures 5.6 and 5.7. This is true both for each subsystem and for the complete system.



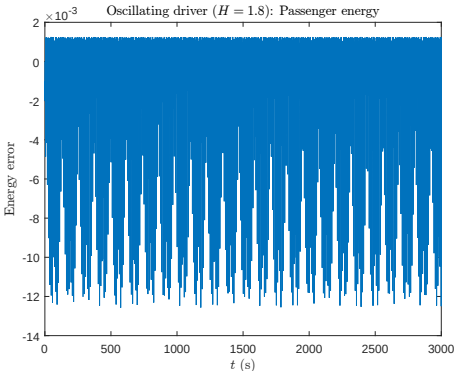
(a) Short term E_d behavior



(c) Long term E_d behavior

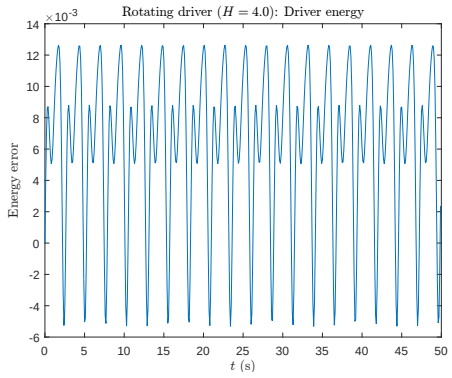


(b) Short term E_p behavior

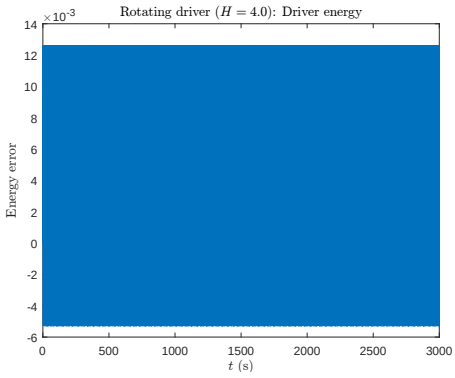


(d) Long term E_p behavior

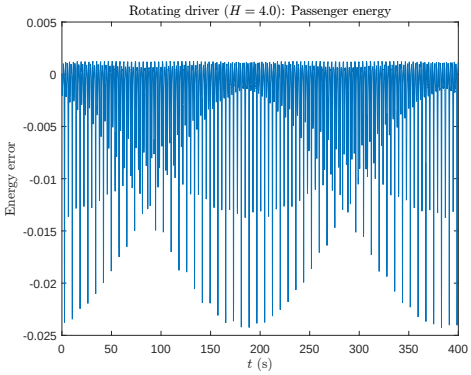
Figure 5.6: Energy behavior of the different subsystems for the oscillating regime ($E_T = 9/5$) with $\epsilon = 1/2$ for the Lobatto-2 method.



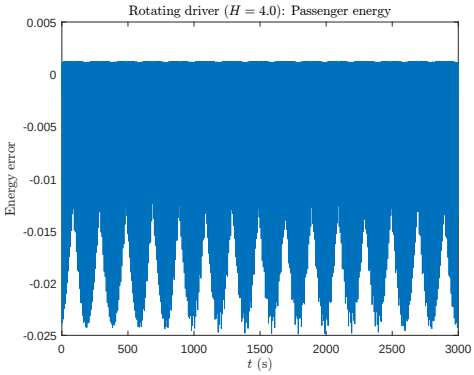
(a) Short term E_d behavior



(c) Long term E_d behavior



(b) Short term E_p behavior



(d) Long term E_p behavior

Figure 5.7: Energy behavior of the different subsystems for the rotating regime ($E_T = 4$) with $\epsilon = 1/2$ for the Lobatto-2 method.

5.6.3 A Fully Chaotic nonholonomic System

Our configuration manifold in this case is $Q = \mathbb{R}^n$, with $n = 2m + 1$ and $m \geq 2$. The corresponding Lagrangian and constraint functions for this system are [see MP06]

$$L(\vec{\mathbf{q}}, \vec{\mathbf{v}}) = \frac{1}{2} \|\vec{\mathbf{v}}\|_2^2 - \frac{1}{2} \left(\|\vec{\mathbf{q}}\|_2^2 + q_{m+2}^2 q_{m+3}^2 + \sum_{i=1}^{m} q_{1+i}^2 q_{m+1+i}^2 \right),$$

$$\Phi(\vec{\mathbf{q}}, \vec{\mathbf{v}}) = v_1 + \sum_{i=m+2}^{n} q_i v_i.$$

This is a chaotic system displaying some strange behavior. As Φ is linear in the velocities, the continuous system must preserve energy and one would expect the discrete system to neatly oscillate around that energy. Numerical results show otherwise, where the energy seems to perform a random walk and its mean squared error for ensembles of initial conditions on the same energy sheet appears to grow with time.

We performed numerical tests following those of [Jay09], where $m = 3$ ($n = 7$) and ensembles of initial conditions with $E_0 = 3.06$,

$$\vec{\mathbf{q}}_0(j, J) = (\alpha(j, J), 0.6, 0.4, 0.2, 1, 1, 1), \quad \vec{\mathbf{v}}_0(j, J) = (0, \beta(j, J), 0, 0, 0, 0, 0),$$

where $\alpha(j, J) = \cos(j\pi/(2J))$, $\beta(j, J) = \sin(j\pi/(2J))$ and $j = 0, ..., J$.

The mean squared error of the energy at the k-th step is defined as:

$$\mu(E,k) = \frac{1}{J+1}\sum_{j=0}^{J}(E_{jk} - E_0)^2 \tag{5.49}$$

where E_{jk} is the energy of the particle corresponding to the j-th initial condition measured at time step k.

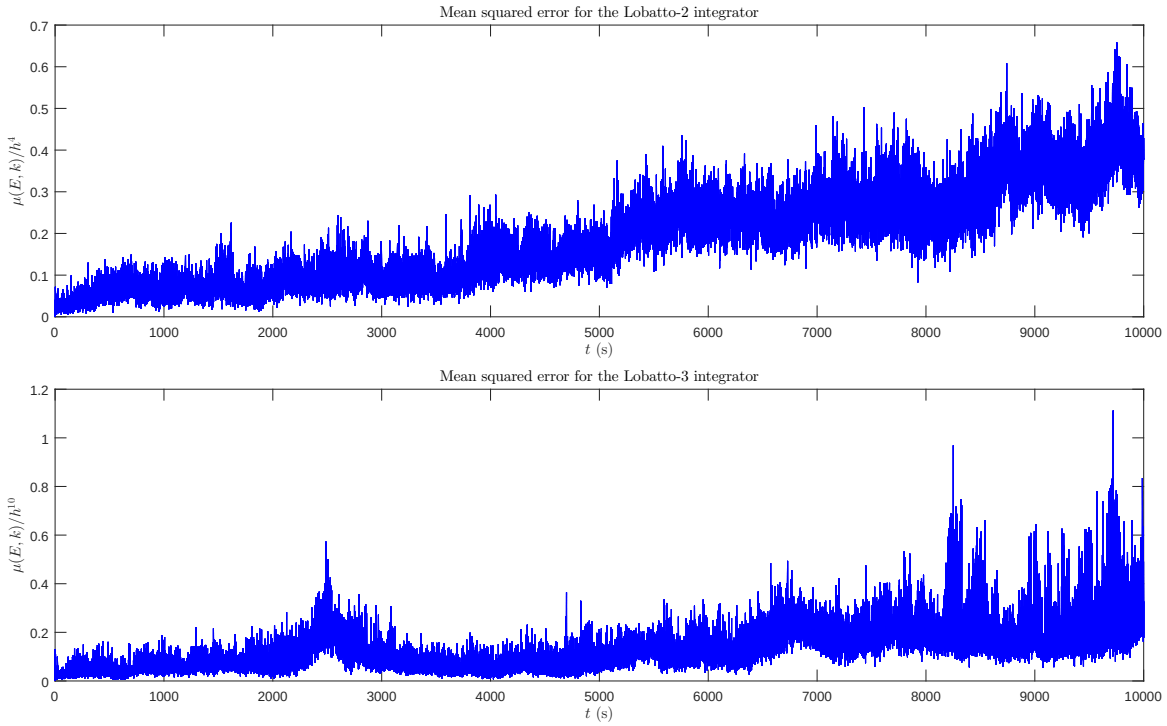


Figure 5.8: $\mu(E,k)/h^4$ and $\mu(E,k)/h^{10}$ behavior with time for the Lobatto-2 and Lobatto-3 methods respectively.

Our integrator matches the behavior of other non-energy preserving integrators such as SPARK or DLA with no apparent gain over any of these, but no loss either.

5.6.4 Nonholonomic vertical disc (unicycle) and elastic spring

As a first example of our integrators in the Lie group setting we consider the simple example of a vertical disc subjected to a harmonic potential which can be thought of as an elastic spring binding it to the origin. In this case $Q = SE(2)$ and the Lagrangian and constraint functions are:

$$L(x,y,\theta,v_x,v_y,v_\theta) = \frac{1}{2}\left[m(v_x^2+v_y^2) + I_z v_\theta^2\right] - \frac{1}{2}(x^2+y^2),$$
$$\Phi(x,y,\theta,v_x,v_y,v_\theta) = v_y\cos\theta - v_x\sin\theta.$$

These can be left-trivialized so that our velocity phase space becomes $SE(2)\times\mathfrak{se}(2)$:

$$\ell(x,y,\theta,v_1,v_2,\omega) = \frac{1}{2}\left[m(v_1^2+v_2^2) + I_z\omega^2\right] - \frac{1}{2}(x^2+y^2),$$
$$\phi(x,y,\theta,v_1,v_2,\omega) = v_2.$$

For the discretization, the cay map was used. As can be seen in fig. 5.9, the numerical order obtained coincides with the expected one.

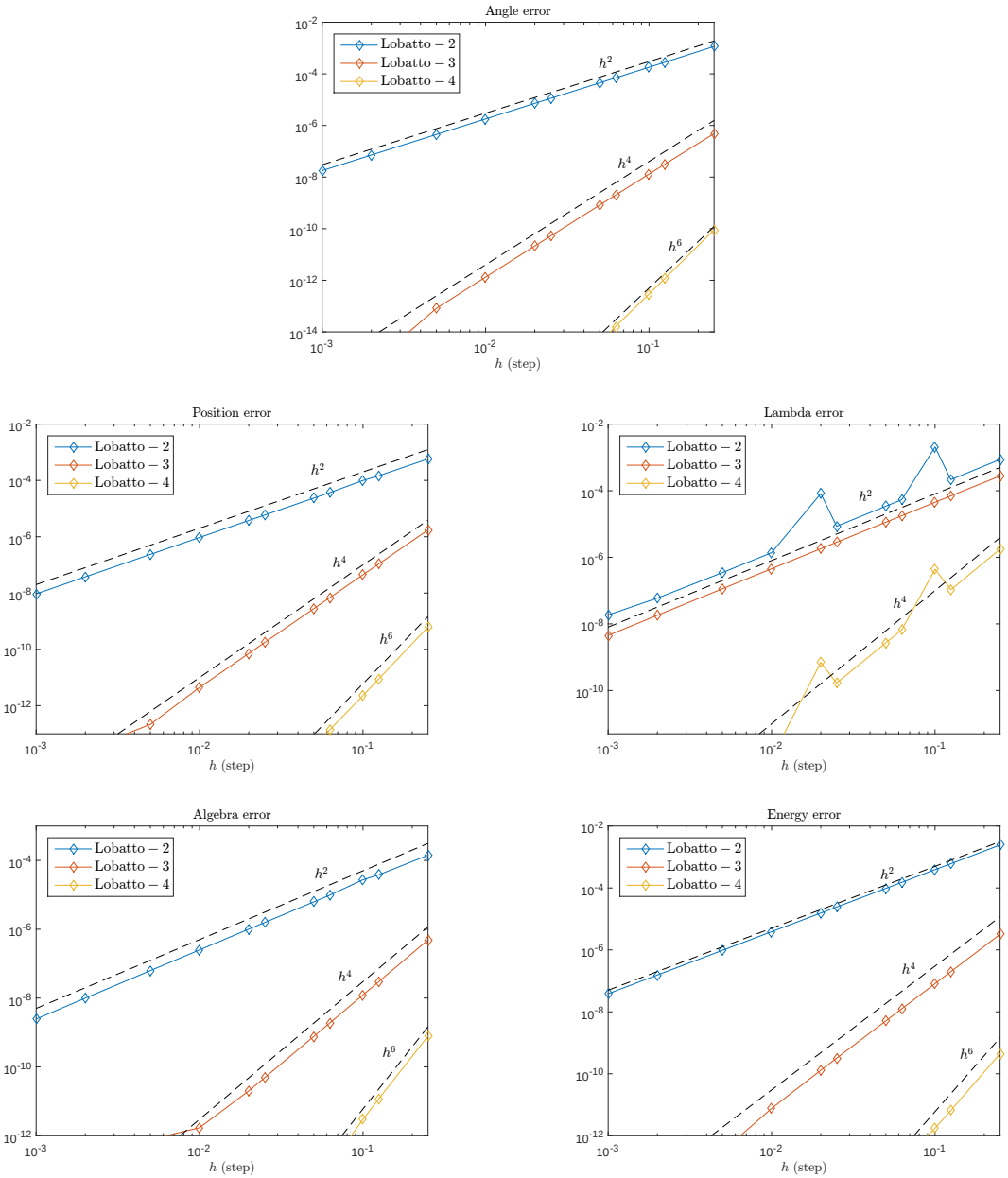


Figure 5.9: Relative error w.r.t. reference values obtained for $h =$ `1e-4` for integrators of various orders. As can be seen, the behavior of the Lagrange multipliers differs from the other variables, as predicted.

5.6.5 Nonholonomic ball on a turntable

As a second and final example in the Lie group setting we consider the classic example of a ball rolling without slipping on a turntable that rotates with constant angular velocity. In this case $Q = SO(3) \times \mathbb{R}^2$ and the left-trivialized Lagrangian and constraint functions are:

$$\ell(\phi, \theta, \psi, x, y, \omega_\xi, \omega_\eta, \omega_\zeta, v_x, v_y) = \frac{1}{2}\left(v_x^2 + v_y^2\right) + \frac{r^2}{2}\left(a\omega_\xi^2 + b\omega_\eta^2 + c\omega_\zeta^2\right),$$
$$\phi_1(\phi, \theta, \psi, x, y, \omega_\xi, \omega_\eta, \omega_\zeta, v_x, v_y) = v_x + \Omega y - r\omega_\eta,$$
$$\phi_2(\phi, \theta, \psi, x, y, \omega_\xi, \omega_\eta, \omega_\zeta, v_x, v_y) = v_y - \Omega x + r\omega_\xi,$$

where ξ, η, ζ are the principal axes of the ball and a, b and c are rescaled moments of inertia.

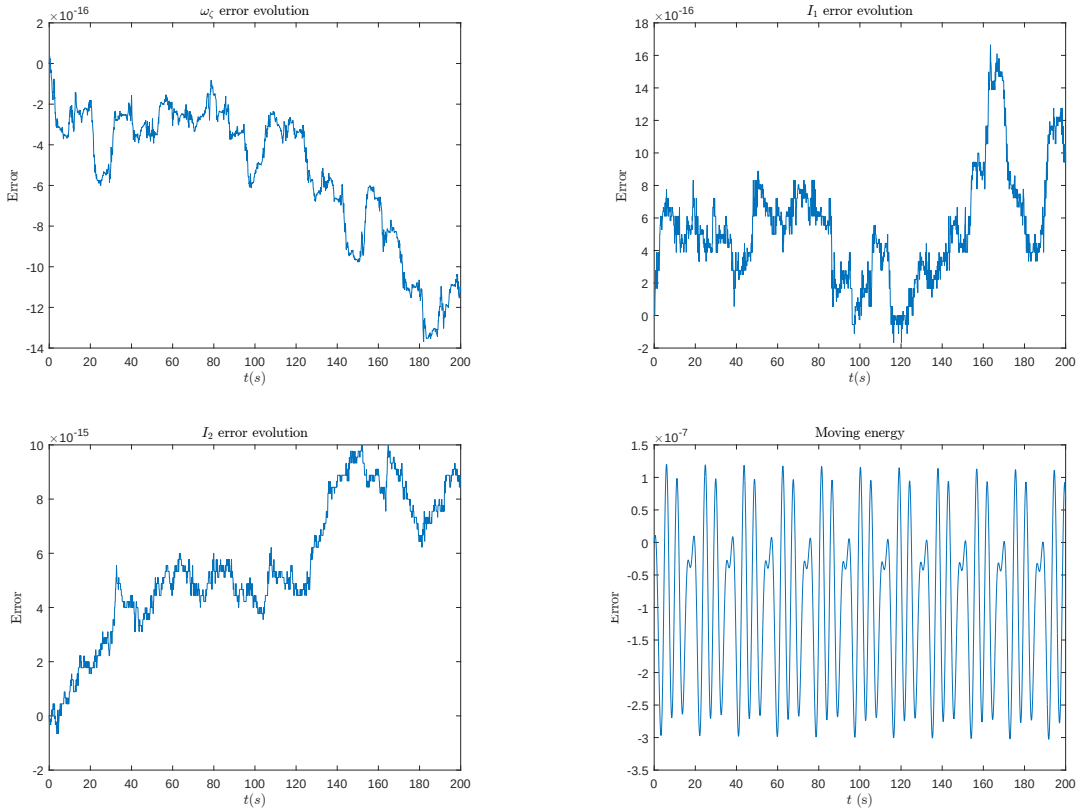


Figure 5.10: Error evolution of the four first integrals. As noted, for the first three the error is introduced by the solver and is in fact lower than the tolerance set for the chosen one (`fsolve` in MATLAB with `TolX = 1e-12`). The behavior of the moving energy is similar to that of the energy of a regular holonomic system. The simulation corresponds to a Lobatto-3 implementation with $\tau = \mathrm{cay}$.

The homogeneous case, where $a = b = c$, is of special interest as it displays periodic motion, implying the existence of $\dim Q - 1 = 4$ first integrals [FS16; FGS18]. The following three,

$$\omega_\zeta, \quad r\omega_\xi - \frac{\Omega}{1+a}x, \quad r\omega_\eta - \frac{\Omega}{1+a}y,$$

are preserved by the integrator, but unless carefully implemented the numerical solver will introduce error (see fig. 5.10). The fourth, dubbed the *moving energy* of the ball,

$$\frac{1}{2}\left(v_x^2 + v_y^2\right) + \frac{ar^2}{2}\left(\omega_\xi^2 + \omega_\eta^2 + \omega_\zeta^2\right) + r\Omega\left(x\omega_\xi + y\omega_\eta\right) - \Omega^2\left(x^2 + y^2\right)$$

displays the sort of behavior one expects from the energy of a holonomic system.

5.7 Numerical optimal control of nonholonomic mechanical systems

In this last section we are going to discuss how to apply our method to optimal control problems.

First, we will discuss how to set up an optimal control problem for a mechanical system and solve it both in the continuous and discrete setting by applying variational integrators for forced systems. Then we will discuss how to tackle nonholonomic case.

5.7.1 Optimal control in the mechanical setting

An optimal control problem for a mechanical system is an optimal control problem where the dynamical system (plant) stems from a mechanical system [see, for instance, Blo15; Cor+02; Kob14; Col+15; KM97]. A problem can be either a purely kinematic problem, where the velocities play the role of controls, or a dynamic problem, where controls appear as force terms. We will focus only on the latter.

Assume we have a regular forced Lagrangian mechanical system (Q, L, f^L). Let us introduce a control space $U \cong \mathbb{R}^r$, $1 \leq r \leq n$, with local coordinates (u^i). A control force is a force $f^U : TQ \times U \to T^*Q$. If we wish to transform our forced Lagrangian mechanical system into a control system, we just need to add the control forces as new forces, so we end up with a new force $f = f^L + f^U$, which will itself be a control force. Applying the Lagrange-D'Alembert principle, we get that the dynamical equations of the system are

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = f_i(q(t), \dot{q}(t), u(t))\,.$$

If $r = n$ and if the Jacobian matrix

$$\left(\frac{\partial f_i}{\partial u_j}\right)$$

is invertible, then the system is said to be fully actuated and by the implicit function theorem it is possible to solve for the different controls and obtain functions $u : T^{(2)}Q \to U$. This case admits a special formulation [CFM16] which we will discuss briefly later on, but will not be our main focus.

As we know, Lagrangian vector fields associated with regular Lagrangians are semisprays (SODEs). The same happens for forced Lagrangian systems, and if we consider control forces, the resulting first order differential system in local coordinates $(q^i, v^i, u^i) \in TQ \times U$ can be written as

$$\begin{aligned} \dot{q}^i &= v^i\,, \\ \dot{v}^i &= F^i(q, v, u)\,. \end{aligned} \tag{5.50}$$

Such a dynamical system can be used as control system for an optimal control problem (see 2.2.5). If we introduce a cost functional and boundary conditions, we can pose an optimal control problem of the same form as 2.11. In particular, assume we have a cost functional with cost function $C : TQ \times U \to \mathbb{R}$ and no terminal costs:

$$\mathcal{J}[c] = \int_{t_a}^{t_b} C(q(t), v(t), u(t))\mathrm{d}t\,. \tag{5.51}$$

Assume also that we have a simple set of boundary values $q(t_a) = q_a$, $v(t_a) = v_a$, $q(t_b) = q_b$, $v(t_b) = v_b$, and fixed t_a and t_b, so we can define the following space of curves,

$$\begin{aligned} &CC((q_a, v_a), (q_b, v_b), [t_a, t_b]) = \\ &\quad \big\{ c : [t_a, t_b] \to TQ \times U \,|\, \mathrm{pr}_{TQ}(c) \in C^2([t_a, t_b]), \mathrm{pr}_U(c) \in C^1([t_a, t_b]), \\ &\quad (\mathrm{pr}_{TQ}(c))(t_a) = (q_a, v_a), (\mathrm{pr}_{TQ}(c))(t_b) = (q_b, v_b) \big\}\,, \end{aligned}$$

with $\text{pr}_{TQ} : TQ \times U \to TQ$ and $\text{pr}_U : TQ \times U \to U$.

Then, the optimal control problem becomes

$$\begin{aligned} &\text{Find } c \in CC((q_a, v_a), (q_b, v_b), [t_a, t_b]) \text{ such that } \min_c \mathcal{J}[c] \\ &\text{subject to:} \\ &\dot{q}^i = v^i \\ &\dot{v}^i = F^i(q, v, u)\,. \end{aligned}$$

The necessary conditions for a given curve $c \in CC((q_a, v_a), (q_b, v_b), [t_a, t_b])$ to be a solution of the optimal control problem are that c is such that the total variations of the following extended cost functional vanish:

$$\begin{aligned} \bar{\mathcal{J}}[\bar{c}] &= \int_{t_a}^{t_b} [C(q(t), v(t), u(t)) + \langle (\mu_q(t), \mu_v(t)), (\dot{q}(t) - v(t), \dot{v}(t) - F(q(t), v(t), u(t)))\rangle]\,\mathrm{d}t \\ &= \int_{t_a}^{t_b} [C(q(t), v(t), u(t)) + \langle \mu_q(t), \dot{q}(t) - v(t)\rangle + \langle \mu_v(t), \dot{v}(t) - F(q(t), v(t), u(t))\rangle]\,\mathrm{d}t \end{aligned}$$

where now $\bar{c} = (q(t), v(t), \mu_q(t), \mu_v(t), u(t))$ is an extended curve on $\mathbb{T}TQ \times U = (TTQ \oplus T^*TQ) \times U$ (similar to what we saw in section 3.1.3). The new variables (μ_q, μ_v) act as Lagrange multipliers, or co-states in the language of optimal control, to enforce the dynamic constraint imposed by the control system.

As t_a and t_b are fixed, the total variations coincide with standard variations. Thus, applying standard calculus of variations we obtain:

$$\begin{aligned} \delta q &: \dot{\mu}_q = \frac{\partial C}{\partial q} - \left\langle \mu_v, \frac{\partial F}{\partial q} \right\rangle \\ \delta v &: \dot{\mu}_v = \frac{\partial C}{\partial v} - \left\langle \mu_v, \frac{\partial F}{\partial v} \right\rangle - \mu_q \\ \delta u &: 0 = \frac{\partial C}{\partial u} - \left\langle \mu_v, \frac{\partial F}{\partial u} \right\rangle \\ \delta \mu_q &: \dot{q} = v \\ \delta \mu_v &: \dot{v} = F(q, v, u)\,. \end{aligned}$$

If the system were fully actuated, it would also be possible to insert $u(q, \dot{q}, \ddot{q})$ in the cost functional of eq.(5.51). This approach leads to an unconstrained, albeit second-order, Lagrangian problem

$$\mathcal{J}[c] = \int_{t_a}^{t_b} C(q, \dot{q}, u(q, \dot{q}, \ddot{q}))\mathrm{d}t = \int_{t_a}^{t_b} \hat{L}(q, \dot{q}, \ddot{q})\mathrm{d}t$$

where now $\hat{L} : T^{(2)}Q \to \mathbb{R}$ is a new second-order Lagrangian / cost function. This is the approach taken in [CFM16]. This approach can be exploited to construct variational integrators using a higher-order Lagrangian formalism. We will not proceed this way and consider only the standard constrained approach.

5.7.2 Discrete optimal control of mechanical systems

The previous derivations are a perfectly valid way to obtain the optimal control dynamics of a mechanical system in the continuous setting. The resulting equations can be integrated with a standard integration algorithm and the boundary value problem (BVP)

posed by the optimal control problem can be solved via a *shooting method* [see Pre+07, chapter 18.1, pg. 959].

As this work is based on the concept of geometric integration, and in particular, variational or pseudo-variational integrators, it makes sense to ask if we can apply a given variational method to the resolution of an mechanical optimal control problem. There are two distinct levels to do so.

The first is to directly discretize eqs.(5.50) and insert them in a discretized version of the cost functional. Applying the discrete Hamilton-Pontryagin principle to the resulting cost functional, we can find the discrete necessary conditions for optimality, which together with the boundary conditions poses a discrete BVP to be solved either in parallel (also known as *relaxation* [see Pre+07, chapter 18.3, pg. 964]) or by shooting. The special case of fully actuated systems is in fact a particular case of this way to proceed.

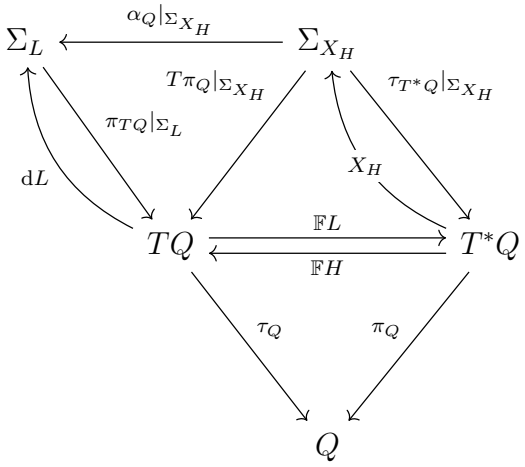
The second way is to use a forced variational integrator to obtain discrete equations of motion for the problem and using these as control system. These are then used as dynamic constraints in a discretized cost functional, preferably using the same quadrature method as the one used for the forcing problem, and again applying the discrete Hamilton-Pontryagin principle. This is the case we are going to consider.

One could ask what the advantage is that we get from using a variational integrator as base dynamics, given that we are in the forced setting. We believe, even if there is no proof as of yet, that, apart from being geometrically correct, forced variational integrators generally have a better long-term energy performance. Moreover, it may be possible that the mechanical control system spends part of the time under no influence of control or force, and during that time the advantage of symplectic methods should be obvious.

To work in this setting, let us first go back to the continuous setting and restate the problem in a more suitable manner and then proceed with the discrete setting.

Continuous optimal control revisited

Remember from section 3.1.5 that we can see our dynamics as a submanifold $\mathrm{im} \mathrm{d}L = \Sigma_L \subset T^*TQ$. If L is regular, then there exists an associated Hamiltonian H and the previous submanifold can be seen as the image by α_Q of the associated submanifold formed by the image of the Hamiltonian vector field X_H, $\mathrm{im} X_H = \Sigma_{X_H} \subset TT^*Q$, that is $\alpha_Q(\Sigma_L) = \Sigma_{X_H}$.



Therefore, we can think of our dynamics as a section of the bundle $T\pi_Q : TT^*Q \to TQ$. This is precisely how the Hamilton-Pontryagin principle works in mechanics: If we take a

curve $\gamma : \mathbb{R} \to TQ$, pass it through $\mathbb{F}L$ and take its tangent lift, the differential equations that it must satisfy to be a critical point of $\mathcal{J}_{\mathcal{HP}}$ (see section 3.1.3) are

$$(q, p = D_2L(q, v), \dot{q} = v, \dot{p} = D_1L(q, v)) .$$

We will call such curves **mechanical curves**.

In the controlled setting we are dealing with mechanical curves on an extended bundle $T\pi_Q^U : TT^*Q \times U \to TQ \times U$ satisfying

$$(q, p(q, v), v, F(q, v, u), u) = (q, D_2L(q, v), v, D_1L(q, v) + f(q, v, u), u) .$$

Thus, let us consider curves $\bar{c} = (q, p, \xi_q, \xi_p, \mu_q, \mu_p, u) : [0, T] \subset \mathbb{R} \to \mathbb{T}T^*Q \times U$, with fixed boundary values $(q(0), p(0)) = (q_a, p_a)$, $(q(T), p(T)) = (q_b, p_b)$, and an extended cost functional, using local coordinates $(q, p, \xi_q, \xi_p, \mu_q, \mu_p, u) \in \mathbb{T}T^*Q \times U$

$$\bar{\mathcal{J}}[\bar{c}] = \int_0^T \left[C(q(t), \xi_q(t), u(t)) + \langle (\mu_q(t), \mu_p(t)) , (\dot{q}(t) - \xi_q(t), \dot{p}(t) - \xi_p(t)) \rangle\right] \mathrm{d}t .$$

We must impose that these curves project onto an extended mechanical curve $(q, p(q, v), v, F(q, v, u), u) \in TT^*Q \times U$. Note that now $(\mu_q, \mu_p) \in T^*_{(q,p)}T^*Q$, instead of being elements in $T^*_{(q,v)}TQ$.

The necessary conditions for optimality are then

$$\begin{aligned}
\dot{\mu}_q + \langle \dot{\mu}_p, D_1p(q, v) \rangle &= D_1C(q, v, u) - \langle \mu_p, D_1F(q, v, u) \rangle , \\
\langle \dot{\mu}_p, D_2p(q, v) \rangle &= D_2C(q, v, u) - \langle \mu_p, D_2F(q, v, u) \rangle - \mu_q , \\
0 &= D_3C(q, v, u) - \langle \mu_p, D_3F(q, v, u) \rangle , \\
\dot{q} &= v, \\
\langle D_1p(q, v), \dot{q} \rangle + \langle D_2p(q, v), \dot{v} \rangle &= F(q, v, u).
\end{aligned}$$

In the continuous setting, so long as the underlying Lagrangian problem is regular we can always go back to the previous formulation in $\mathbb{T}TQ \times U$, but this formulation is specially suitable for the discrete setting where a variationally partitioned method can be readily applied.

Discrete optimal control using variational integrators

Similar to what we did in section 3.2.5, let us use an s-stage RK scheme and its symplectic conjugate, defined by the set of RK coefficients $((a_{ij}, b_j), (\hat{a}_{ij}, \hat{b}_j))$. We can consider the space of *s-stage variationally partitioned RK (s-stage VPRK) sequences*:

$$\begin{aligned}
&CC_d^s((q_a, p_a), (q_b, p_b)) \\
&= \left\{ \left(q, p, \tilde{\mu}_q, \tilde{\mu}_p, \left\{ Q^i, V^i, P^i, \tilde{\mathrm{M}}_q^i, \tilde{\mathrm{M}}_p^i, U^i \right\}_{i=1}^s \right) : T_d \to T^*T^*Q \times ((T^* (T^*Q) \times_Q TQ) \times U)^s \mid \right. \\
&\left. (q(a), p(a)) = (q_a, p_a), (q(b), p(b)) = (q_b, p_b) \right\} .
\end{aligned}$$

Then we can define the following functional, $\bar{\mathcal{J}}_d : CC_d^s((q_a,p_a),(q_b,p_b)) \to \mathbb{R}$,

$$\begin{aligned}\bar{\mathcal{J}}_d[\bar{c}_d] = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[& C\left(Q_k^i, V_k^i, U_k^i\right) \\ & + \left\langle \mathrm{M}_{Q,k}^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle + \left\langle \mu_{q,k+1}, \frac{q_{k+1}-q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle \\ & + \left\langle \mathrm{M}_{P,k}^i, \frac{P_k^i - p_k}{h} - \sum_{j=1}^{s} \hat{a}_{ij} \left[F(Q_k^j, V_k^j, U_k^j)\right] \right\rangle \\ & + \left\langle \mu_{p,k+1}, \frac{p_{k+1}-p_k}{h} - \sum_{j=1}^{s} \hat{b}_j \left[F(Q_k^j, V_k^j, U_k^j)\right] \right\rangle \Bigg] .\end{aligned}$$

If we define the set $\{v_k\}_{k=0}^N$ by the relation $p_k = D_2L(q_k, v_k)$, then we can evaluate this functional over an extended mechanical curve satisfying

$$(q, p(q,v), v, F(q,v,u), u) = (q, D_2L(q,v), v, D_1L(q,v) + f(q,v,u), u)$$

and obtain

$$\begin{aligned}\bar{\mathcal{J}}_d[\bar{c}_d] = \sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[& C\left(Q_k^i, V_k^i, U_k^i\right) \\ & + \left\langle \mathrm{M}_{Q,k}^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle + \left\langle \mu_{q,k+1}, \frac{q_{k+1}-q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle \\ & + \left\langle \mathrm{M}_{P,k}^i, \frac{D_2L(Q_k^i, V_k^i) - D_2L(q_k, v_k)}{h} - \sum_{j=1}^{s} \hat{a}_{ij} \left[D_1L(Q_k^j, V_k^j) + f(Q_k^j, V_k^j, U_k^j)\right] \right\rangle \\ & + \left\langle \mu_{p,k+1}, \frac{D_2L(q_{k+1}, v_{k+1}) - D_2L(q_k, v_k)}{h} - \sum_{j=1}^{s} \hat{b}_j \left[D_1L(Q_k^j, V_k^j) + f(Q_k^j, V_k^j, U_k^j)\right] \right\rangle \Bigg]\end{aligned}$$

where we can identify our variationally partitioned integrator as constraints (cf. eq.4.10). Taking variations we can readily obtain the discrete necessary conditions for optimality.

5.7.3 An exploration of continuous optimal control of nonholonomic systems

For simplicity, let us work again in $\mathbb{T}TQ \times U$ formalism. Assume we have a regular and compatible controlled nonholonomic problem (Q, L, N, f, U), with $f : TQ \times U \to T^*Q$. Its equations of motion can be obtained by applying the Chetaev and Lagrange-D'Alembert principles (see defs.5.1.2 and 4.1.1 and [Blo15]), leading to

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\left(\dfrac{\partial L}{\partial \dot{q}^i}\right) - \dfrac{\partial L}{\partial q^i} = \left\langle \lambda, \dfrac{\partial \Phi}{\partial \dot{q}^i} \right\rangle + f_i(q, \dot{q}, u), \quad \text{for } i = 1, ..., n; \\ \Phi(q, \dot{q}) = 0. \end{cases}$$

As we saw in section 5.4.2, in these conditions it must be possible to obtain an expression for $\lambda_\alpha = \kappa_\alpha(q, v, u)$ from the constraint equations. Substituting such κ_α turn

our constrained problem into an equivalent unconstrained forced problem which, if initial conditions are chosen in N, is equivalent to the original problem. In such a case the resulting system can be rewritten in the generic first order form

$$\begin{aligned}\dot{q}^i &= v^i \\ \dot{v}^i &= F^i(q, v, u).\end{aligned}$$

Given a cost function $C : TQ \times U \to \mathbb{R}$, we define a cost functional of the form

$$\begin{aligned}\mathcal{J}[c] &= \int_0^T \left[C(q, v, u) + \langle(\mu_q, \mu_v), (\dot{q} - v, \dot{v} - F(q, v, u))\rangle\right] \mathrm{d}t \\ &= \int_0^T \left[C(q, v, u) + \langle\mu_q, \dot{q} - v\rangle + \langle\mu_v, \dot{v} - F(q, v, u)\rangle\right] \mathrm{d}t\,.\end{aligned}$$

The functional is defined on the space of parametrized curves of $\mathbb{T}TQ \times U$ with fixed ends. This is in essence what most authors do, with some modifications such as using adapted coordinates to the nonholonomic constraint manifold (quasi or pseudovelocities) [e.g. KM97; Col+15; Kob14].

When the forced and controlled system is derived from a nonholonomic system, the forcing term F can be split into two parts,

$$F^i(q, v, u) = F_0^i(q, v, u) + \kappa_\alpha(q, v, u)G^{\alpha,i}(q, v).$$

Variation of the functional then takes the form

$$\begin{aligned}\langle\delta\mathcal{J}[c], \delta c\rangle = \int_0^T \Bigg[&\left\langle\frac{\partial C}{\partial q}, \delta q\right\rangle + \left\langle\frac{\partial C}{\partial v}, \delta v\right\rangle + \left\langle\frac{\partial C}{\partial u}, \delta u\right\rangle \\ &+ \langle\delta\mu_q, \dot{q} - v\rangle + \langle\mu_q, \delta\dot{q} - \delta v\rangle + \langle\delta\mu_v, \dot{v} - F_0 - \kappa_\alpha G^\alpha\rangle \\ &+ \left\langle\mu_v, \delta\dot{v} - \left\langle\frac{\partial F_0}{\partial q}, \delta q\right\rangle - \left\langle\frac{\partial F_0}{\partial v}, \delta v\right\rangle - \left\langle\frac{\partial F_0}{\partial u}, \delta u\right\rangle\right\rangle \\ &- \left\langle\mu_v, \left\langle\frac{\partial\kappa_\alpha}{\partial q}G^\alpha, \delta q\right\rangle + \left\langle\frac{\partial\kappa_\alpha}{\partial v}G^\alpha, \delta v\right\rangle + \left\langle\frac{\partial\kappa_\alpha}{\partial u}G\alpha, \delta u\right\rangle\right\rangle \\ &- \left\langle\mu_v, \left\langle\kappa_\alpha\frac{\partial G^\alpha}{\partial q}, \delta q\right\rangle + \left\langle\kappa_\alpha\frac{\partial G^\alpha}{\partial v}, \delta v\right\rangle\right\rangle\Bigg] \mathrm{d}t\,.\end{aligned}$$

Collecting terms and applying integration by parts we obtain the following variation terms:

$$\begin{aligned}\delta q &: \dot{\mu}_q = \frac{\partial C}{\partial q} - \left\langle\mu_v, \frac{\partial F_0}{\partial q} + \frac{\partial\kappa_\alpha}{\partial q}G^\alpha + \kappa_\alpha\frac{\partial G^\alpha}{\partial q}\right\rangle \\ \delta v &: \dot{\mu}_v = \frac{\partial C}{\partial v} - \left\langle\mu_v, \frac{\partial F_0}{\partial v} + \frac{\partial\kappa_\alpha}{\partial v}G^\alpha + \kappa_\alpha\frac{\partial G^\alpha}{\partial v}\right\rangle - \mu_q \\ \delta u &: 0 = \frac{\partial C}{\partial u} - \left\langle\mu_v, \frac{\partial F_0}{\partial u} + \frac{\partial\kappa_\alpha}{\partial u}G^\alpha\right\rangle \\ \delta\mu_q &: \dot{q} = v \\ \delta\mu_v &: \dot{v} = F_0 - \kappa_\alpha G^\alpha.\end{aligned}$$

These must vanish for the functional to reach a stationary value.

Example 5.7.1. (Nonholonomic controlled particle). Assume the following nonholonomic Lagrangian problem. Let $Q = \mathbb{R}^3$ be our configuration manifold, $U \subset \mathbb{R}^2$ our control space and $N \subset TQ$ the constraint submanifold, and let us use local coordinates (x, y, z, v_x, v_y, v_z) on TQ and (u^1, u^2) on U.

Let $L : TQ \to \mathbb{R}$ and $\Phi : N \to \mathbb{R}$ be the following Lagrangian and constraint functions respectively,

$$\begin{aligned} L(q, v) &= \frac{1}{2}(v_x^2 + v_y^2 + v_z^2), \\ \Phi(q, v) &= v_z - y v_x, \end{aligned}$$

with $\Phi^{-1}(0) = N$.

Finally, consider the control force $f : TQ \times U \to T^*Q$ defined by

$$f(x, y, z, v_x, v_y, v_z, u^1, u^2) = (x, y, z, u^1, u^2, y u^1)\,.$$

Applying the Chetaev and Lagrange-D'Alembert principles and casting the results as a first order system we get:

$$\begin{aligned} \dot{x} &= v_x\,, \\ \dot{y} &= v_y\,, \\ \dot{z} &= v_z\,, \\ \dot{v}_x &= u^1 - \lambda y\,, \\ \dot{v}_y &= u^2\,, \\ \dot{v}_z &= y u^1 + \lambda\,, \\ 0 &= v_z - y v_x\,. \end{aligned}$$

These are the equations of a nonholonomic controlled particle.

This system defines a vector field (a semispray) ξ. In order to determine λ we can simply apply the vector field to the constraint

$$\imath_\xi \mathrm{d}\Phi = \dot{v}_z - \dot{y}\dot{x} - y\dot{v}_x = 0 \Rightarrow \lambda = \kappa(y, v_x, v_y) = \frac{v_x v_y}{1 + y^2}\,.$$

Substituting λ by the expression just found we may insert this in the cost functional corresponding to an optimal control problem with cost function $C : TQ \times U \to \mathbb{R}$,

$$\begin{aligned} \mathcal{J}[c] = \int_0^T \Big[& C(q, v, u) + \mu_x\,(\dot{x} - v_x) + \mu_y\,(\dot{y} - v_y) + \mu_z\,(\dot{x} - v_z) \\ & + \mu_{v_x}\left(\dot{v}_x - u^1 + \frac{v_x v_y}{1 + y^2} y\right) + \mu_{v_y}\left(\dot{v}_y - u^2\right) + \mu_{v_z}\left(\dot{v}_z - u^1 y - \frac{v_x v_y}{1 + y^2}\right)\Big]\,\mathrm{d}t, \end{aligned}$$

and take variations to obtain

$$\begin{aligned}
\delta x &: \dot{\mu}_x = \frac{\partial C}{\partial x},\\
\delta y &: \dot{\mu}_y = \frac{\partial C}{\partial y} + \frac{v_x v_y}{1+y^2}\mu_{v_x} - \mu_{v_z}u^1 + (\mu_{v_z} - y\mu_{v_x})\frac{2yv_xv_y}{(1+y^2)^2},\\
\delta z &: \dot{\mu}_z = \frac{\partial C}{\partial z},\\
\delta v_x &: \dot{\mu}_{v_x} = \frac{\partial C}{\partial v_x} - \mu_x - \frac{v_y}{1+y^2}\left(\mu_{v_z} - y\mu_{v_x}\right),\\
\delta v_y &: \dot{\mu}_{v_y} = \frac{\partial C}{\partial v_y} - \mu_y - \frac{v_x}{1+y^2}\left(\mu_{v_z} - y\mu_{v_x}\right),\\
\delta v_z &: \dot{\mu}_{v_z} = \frac{\partial C}{\partial v_z} - \mu_z,\\
\delta u^1 &: \frac{\partial C}{\partial u^1} = \mu_{v_x} + y\mu_{v_z},\\
\delta u^2 &: \frac{\partial C}{\partial u^2} = \mu_{v_y}
\end{aligned}$$

together with the dynamical equations derived from the rest of the variations.

Assume that we have the cost function

$$C(q,v,u) = \frac{1}{2}(u_1^2 + u_2^2)\,. \tag{5.52}$$

An optimal control problem could be to minimize the cost functional subject to the dynamics of the nonholonomic controlled particle such that $q(0) = q_0$, $v(0) = v_0$, $q(T) = q_T$, $v(T) = v_T$. In order to solve the problem we would need to solve the BVP defined by these conditions together with the necessary conditions for optimality

$$\begin{aligned}
\delta x &: \dot{\mu}_x = 0,\\
\delta y &: \dot{\mu}_y = \frac{v_x v_y}{1+y^2}\mu_{v_x} - \mu_{v_z}u^1 + (\mu_{v_z} - y\mu_{v_x})\frac{2yv_xv_y}{(1+y^2)^2},\\
\delta z &: \dot{\mu}_z = 0,\\
\delta v_x &: \dot{\mu}_{v_x} = -\mu_x - \frac{v_y}{1+y^2}\left(\mu_{v_z} - y\mu_{v_x}\right),\\
\delta v_y &: \dot{\mu}_{v_y} = -\mu_y - \frac{v_x}{1+y^2}\left(\mu_{v_z} - y\mu_{v_x}\right),\\
\delta v_z &: \dot{\mu}_{v_z} = -\mu_z,\\
\delta u^1 &: u^1 = \mu_{v_x} + y\mu_{v_z},\\
\delta u^2 &: u^2 = \mu_{v_y}.
\end{aligned}$$

Remark. Note that this system is actually underdetermined due to the fact that we have 2 controls and 3 co-states. In order to have a fully determined system we should have removed either the equations for v_x or for v_z, which in turn eliminates one of the associated co-states, but for clarity's sake it is better to work like this. In this case, we can fully determine the system by adding an additional constraint, such as asking for $(\mu_{v_x}, \mu_{v_y}, \mu_{v_z})$ to satisfy

$$\min_{(\mu_{v_x},\mu_{v_y},\mu_{v_z})} \frac{1}{2}(\mu_{v_x}^2(T) + \mu_{v_y}^2(T) + \mu_{v_z}^2(T))\,.$$

Either way, the resulting control law, which is what we are after, is exactly the same. △

Now we would like to work with κ_α as independent variables to be determined together with the rest of the variables of the system. This is important for the discrete case, as in general obtaining an explicit expression for the discrete values of λ is a daunting task, as it is not true that $\Lambda_k^i = \kappa(Q_k^i, V_k^i, U_k^i)$ in general.

The first strategy one can try is to insert a new constraint term in the functional to account for the nonholonomic constraint on the underlying mechanical system:

$$\langle \mu_{\lambda,\alpha}, \Phi^\alpha(q,v) \rangle \,.$$

Variation of this new term leads to

$$\langle \delta\mu_{\lambda,\alpha}, \Phi^\alpha \rangle + \left\langle \mu_{\lambda,\alpha}, \frac{\partial \Phi^\alpha}{\partial q}\delta q + \frac{\partial \Phi^\alpha}{\partial v}\delta v \right\rangle,$$

which, combined with the rest of the functional, take the form

$$\begin{aligned}
\delta q : \dot{\mu}_q &= \frac{\partial C}{\partial q} - \left\langle \mu_v, \frac{\partial F_0}{\partial q} + \lambda_\alpha \frac{\partial G^\alpha}{\partial q} \right\rangle + \left\langle \mu_{\lambda,\alpha}, \frac{\partial \Phi^\alpha}{\partial q} \right\rangle \\
\delta v : \dot{\mu}_v &= \frac{\partial C}{\partial v} - \left\langle \mu_v, \frac{\partial F_0}{\partial v} + \lambda_\alpha \frac{\partial G^\alpha}{\partial v} \right\rangle + \left\langle \mu_{\lambda,\alpha}, \frac{\partial \Phi^\alpha}{\partial v} \right\rangle - \mu_q \\
\delta u : 0 &= \frac{\partial C}{\partial u} - \left\langle \mu_v, \frac{\partial F_0}{\partial u} \right\rangle \\
\delta \lambda_\alpha : 0 &= \left\langle \mu_v, \frac{\partial G^\alpha}{\partial v} \right\rangle \\
\delta \mu_q : \dot{q} &= v \\
\delta \mu_v : \dot{v} &= F_0 - \lambda_\alpha G^\alpha \\
\delta \mu_{\lambda,\alpha} : 0 &= \Phi^\alpha(q,v),
\end{aligned}$$

which must vanish for the functional to be stationary.

Do these two different sets of variations lead to the same stationary values? The answer is negative. This latter set of equations is far more restrictive than the former, mainly due to the variations in λ_α, which lead to a constraint on μ_v. This is not present in the former, which in turn leads to better extremal values.

Example 5.7.1. (Nonholonomic controlled particle, continued). Let us work with λ as free independent variables and add the constraint to the action. The resulting

equations are:

$$\begin{aligned}
\delta x &: \dot{\mu}_x = \frac{\partial C}{\partial x}, \\
\delta y &: \dot{\mu}_y = \frac{\partial C}{\partial y} + \mu_{v_x}\lambda - \mu_{v_z}u^1 - \mu_\lambda v_x, \\
\delta z &: \dot{\mu}_z = \frac{\partial C}{\partial z}, \\
\delta v_x &: \dot{\mu}_{v_x} = \frac{\partial C}{\partial v_x} - \mu_x - \mu_\lambda y, \\
\delta v_y &: \dot{\mu}_{v_y} = \frac{\partial C}{\partial v_y} - \mu_y, \\
\delta v_z &: \dot{\mu}_{v_z} = \frac{\partial C}{\partial v_z} - \mu_z + \mu_\lambda, \\
\delta \lambda &: \mu_{v_z} - y\mu_{v_x}, \\
\delta u^1 &: \frac{\partial C}{\partial u^1} = \mu_{v_x} + y\mu_{v_z}, \\
\delta u^2 &: \frac{\partial C}{\partial u^2} = \mu_{v_y}
\end{aligned}$$

together with the dynamical equations and the constraint. Clearly, these equations are not equivalent to the ones previously obtained.

Another strategy we may try is to impose variations on $\delta\lambda_\alpha$. As it turns out, this is the way to go and a method that can be applied to the discrete case, but not in a straightforward manner.

In the continuous case this just means that we would need to make the substitution $\delta\lambda_\alpha \mapsto \frac{\partial \kappa_\alpha}{\partial q}\delta q + \frac{\partial \kappa_\alpha}{\partial v}\delta v + \frac{\partial \kappa_\alpha}{\partial u}\delta u$, which leads to the correct variation terms. Finally, one just needs to add the constraint equations to the resulting equations of motion to close the system.

The fact that the partial derivatives of $\kappa_\alpha(q, v, u)$ show up might make it look like we did not solve the problem at all, but in fact this is sufficient for us to work in the discrete case, as we do not need the functions themselves but its derivatives.

Still, this cannot be applied directly to the discrete case for reasons that will be discussed later. The best way to apply this is to use additional Lagrange multipliers, which in the continuous realm may look absolutely unnecessary. Let us recast the first cost functional as

$$\begin{aligned}
\hat{\mathcal{J}}[c] = \int_0^T \big[& C(q, v, u) + \langle \mu_q, \dot{q} - v \rangle \\
& + \langle \mu_v, \dot{v} - F_0(q, v, u) - \lambda_\alpha G^\alpha(q, v) \rangle + \langle \mu_\lambda^\alpha, \lambda_\alpha - \kappa_\alpha(q, v, u) \rangle \big] \, \mathrm{d}t \, .
\end{aligned}$$

Let us take variations of the cost functional

$$\begin{aligned}\left\langle \delta\hat{\mathcal{J}}[c], \delta c\right\rangle = \int_0^T \Bigg[&\left\langle \frac{\partial C}{\partial q}, \delta q\right\rangle + \left\langle \frac{\partial C}{\partial v}, \delta v\right\rangle + \left\langle \frac{\partial C}{\partial u}, \delta u\right\rangle \\ &+ \langle \delta\mu_q, \dot{q} - v\rangle + \langle \mu_q, \delta\dot{q} - \delta v\rangle + \langle \delta\mu_v, \dot{v} - F_0 - \lambda_\alpha G^\alpha\rangle \\ &+ \left\langle \mu_v, \delta\dot{v} - \left\langle \frac{\partial F_0}{\partial q}, \delta q\right\rangle - \left\langle \frac{\partial F_0}{\partial v}, \delta v\right\rangle - \left\langle \frac{\partial F_0}{\partial u}, \delta u\right\rangle\right\rangle \\ &- \left\langle \mu_v, \left\langle \lambda_\alpha \frac{\partial G^\alpha}{\partial q}, \delta q\right\rangle + \left\langle \lambda_\alpha \frac{\partial G^\alpha}{\partial v}, \delta v\right\rangle\right\rangle \\ &- \langle \mu_v, \delta\lambda_\alpha g^\alpha\rangle + \langle \delta\mu_\lambda^\alpha, \lambda_\alpha - \kappa_\alpha\rangle \\ &+ \left\langle \mu_\lambda^\alpha, \delta\lambda_\alpha - \left\langle \frac{\partial \kappa_\alpha}{\partial q}, \delta q\right\rangle - \left\langle \frac{\partial \kappa_\alpha}{\partial v}, \delta v\right\rangle - \left\langle \frac{\partial \kappa_\alpha}{\partial u}, \delta u\right\rangle\right\rangle\Bigg] \mathrm{d}t\,.\end{aligned}$$

The corresponding variations are

$$\begin{aligned}\delta q &: \dot{\mu}_q = \frac{\partial C}{\partial q} - \left\langle \mu_v, \frac{\partial F_0}{\partial q} + \lambda_\alpha \frac{\partial G^\alpha}{\partial q}\right\rangle - \left\langle \mu_\lambda^\alpha, \frac{\partial \kappa_\alpha}{\partial q}\right\rangle \\ \delta v &: \dot{\mu}_v = \frac{\partial C}{\partial v} - \left\langle \mu_v, \frac{\partial F_0}{\partial v} + \lambda_\alpha \frac{\partial G^\alpha}{\partial v}\right\rangle - \left\langle \mu_\lambda^\alpha, \frac{\partial \kappa_\alpha}{\partial v}\right\rangle - \mu_q \\ \delta u &: 0 = \frac{\partial C}{\partial u} - \left\langle \mu_v, \frac{\partial F_0}{\partial u}\right\rangle - \left\langle \mu_\lambda^\alpha, \frac{\partial \kappa_\alpha}{\partial u}\right\rangle \\ \delta\lambda_\alpha &: \mu_\lambda^\alpha = \langle \mu_v, g^\alpha\rangle \\ \delta\mu_q &: \dot{q} = v \\ \delta\mu_v &: \dot{v} = F_0 - \lambda_\alpha G^\alpha \\ \delta\mu_\lambda^\alpha &: \lambda_\alpha = \kappa_\alpha\end{aligned}$$

and it is evident that the equations are equivalent to the first set we derived. Thus, as we stated above, if we restrict to initial and final conditions in N, it is perfectly possible for us to exchange the equations obtained from $\delta\mu_\lambda^\alpha$ to

$$\Phi^\alpha(q, v) = 0,$$

which equally determines the different values of λ_α. Thus, κ_α is not needed anymore, and only its derivatives suffice to solve the problem.

Example 5.7.1. (Nonholonomic controlled particle, continued). Finally, let us work with λ as independent variables but impose constraints on its variations. To obtain said constraints it suffices to obtain the dynamical system the variations must satisfy, i.e.

$$\begin{aligned}\delta\dot{x} &= \delta v_x \\ \delta\dot{y} &= \delta v_y \\ \delta\dot{z} &= \delta v_z \\ \delta\dot{v}_x &= \delta u^1 - \delta\lambda y - \lambda\delta y \\ \delta\dot{v}_y &= \delta u^2 \\ \delta\dot{v}_z &= \delta y u^1 + y\delta u^1 + \delta\lambda \\ 0 &= \delta v_z - \delta y v_x - y\delta v_x\,.\end{aligned}$$

Differentiating the constraint equation w.r.t. time, we get $\delta\dot{v}_z - \delta\dot{y}v_x - \delta y\dot{v}_x - \dot{y}\delta v_x - y\delta\dot{v}_x$, which after substitution of the rest of the equations inside it, lead to

$$\delta\lambda = \frac{1}{1+y^2}\left(v_y\delta v_x + v_x\delta v_y - 2y\lambda\delta y\right).$$

Introducing this constraint, the equations for the optimal control problem become:

$$\begin{aligned}
\delta x &: \dot{\mu}_x = \frac{\partial C}{\partial x},\\
\delta y &: \dot{\mu}_y = \frac{\partial C}{\partial y} + \mu_{v_x}\lambda - \mu_{v_z}u^1 + \mu_\lambda\frac{2y\lambda}{1+y^2},\\
\delta z &: \dot{\mu}_z = \frac{\partial C}{\partial z},\\
\delta v_x &: \dot{\mu}_{v_x} = \frac{\partial C}{\partial v_x} - \mu_x - \mu_\lambda\frac{v_y}{1+y^2},\\
\delta v_y &: \dot{\mu}_{v_y} = \frac{\partial C}{\partial v_y} - \mu_y - \mu_\lambda\frac{v_x}{1+y^2},\\
\delta v_z &: \dot{\mu}_{v_z} = \frac{\partial C}{\partial v_z} - \mu_z,\\
\delta\lambda &: \mu_\lambda = \mu_{v_z} - y\mu_{v_x},\\
\delta u^1 &: \frac{\partial C}{\partial u^1} = \mu_{v_x} + y\mu_{v_z},\\
\delta u^2 &: \frac{\partial C}{\partial u^2} = \mu_{v_y}
\end{aligned}$$

together with the dynamical equations and either $\lambda = \kappa(q,v,u)$ or the nonholonomic constraint. This time the equations are indeed equivalent to those of the first system, as can be readily checked.

5.7.4 Discrete optimal control of nonholonomic systems

In order to apply our nonholonomic integrator it is again necessary to recast the continuous problem as an optimal control problem on the bundle $\pi : \mathbb{T}T^*Q\times T^*\Lambda\times U \to TQ\times\Lambda\times U$ over an extended mechanical curve satisfying

$$\begin{aligned}
&(q, p(q,v), v, F(q,v,u,\lambda), \lambda, \mu_q, \mu_p, \mu_\lambda, u) =\\
&\qquad (q, D_2L(q,v), v, D_1L(q,v) + \langle\lambda, D_2\Phi(q,v)\rangle\, f(q,v,u), \lambda, , \mu_q, \mu_p, \mu_\lambda, u)\,.
\end{aligned}$$

This leads us the extended cost functional

$$\begin{aligned}
\bar{\mathcal{J}}[\bar{c}] = \int_0^T \big[&C(q(t),v(t),u(t)) + \langle(\mu_q,\mu_p)\,, (\dot{q}-v, (p(q,v))^{\cdot} - F(q,v,u,\lambda))\rangle\\
&+ \langle\mu_\lambda, \lambda - \kappa(q,v,u)\rangle\big]\,\mathrm{d}t\,.
\end{aligned}$$

Taking variations we obtain the necessary conditions for optimality

$$\begin{aligned}
\dot{\mu}_q + \langle \dot{\mu}_p, D_1 p(q,v)\rangle &= D_1 C(q,v,u) - \langle \mu_p, D_1 F(q,v,u,\lambda)\rangle - \langle \mu_\lambda, D_1\kappa(q,v,u)\rangle\,,\\
\langle \dot{\mu}_p, D_2 p(q,v)\rangle &= D_2 C(q,v,u) - \langle \mu_p, D_2 F(q,v,u,\lambda)\rangle - \langle \mu_\lambda, D_2\kappa(q,v,u)\rangle - \mu_q,\\
0 &= D_3 C(q,v,u) - \langle \mu_p, D_3 F(q,v,u,\lambda)\rangle - \langle \mu_\lambda, D_3\kappa(q,v,u)\rangle\,,\\
0 &= \mu_\lambda - \langle \mu_p, D_4 F(q,v,u,\lambda)\rangle\,,\\
\dot{q} &= v,\\
\langle D_1 p(q,v), \dot{q}\rangle + \langle D_2 p(q,v), \dot{v}\rangle &= F(q,v,u,\lambda),\\
\lambda &= \kappa(q,v,u)\,.
\end{aligned}$$

As before, the last equation can be substituted by the constraint so long as we restrict to initial and terminal conditions in N.

This formulation can be used as the basis for the discrete setting. What remains is to obtain the discrete equivalents of the derivatives of κ. We can obtain these in the following manner.

First, consider the equations of our forced and controlled nonholonomic integrator:

$$\begin{aligned}
q_{k+1} &= q_k + h\sum_{i=1}^{s} b_i V_k^i,\\
Q_k^i &= q_k + h\sum_{j=1}^{s} a_{ij} V_k^j,\\
q_k^i &= Q_k^i,\\
D_2L(q_{k+1},v_{k+1}) &= D_2L(q_k,v_k)\\
&\quad + h\sum_{i=1}^{s} \hat{b}_i \left[D_1L(Q_k^j,V_k^j) + \left\langle \Lambda_k^j, D_2\Phi(Q_k^j,V_k^j)\right\rangle + f(Q_k^j,V_k^j,U_k^j)\right],\\
D_2L(Q_k^i,V_k^i) &= D_2L(q_k,v_k)\\
&\quad + h\sum_{j=1}^{s} \hat{a}_{ij} \left[D_1L(Q_k^j,V_k^j) + \left\langle \Lambda_k^j, D_2\Phi(Q_k^j,V_k^j)\right\rangle + f(Q_k^j,V_k^j,U_k^j)\right],\\
D_2L(q_k^i,v_k^i) &= D_2L(q_k,v_k)\\
&\quad + h\sum_{j=1}^{s} a_{ij} \left[D_1L(Q_k^j,V_k^j) + \left\langle \Lambda_k^j, D_2\Phi(Q_k^j,V_k^j)\right\rangle + f(Q_k^j,V_k^j,U_k^j)\right],\\
0 &= \Phi(q_k^i,v_k^i).
\end{aligned}$$

Without any other consideration, the controls, which only appear as inner stage variables $\{U_k^i\}_{i=1}^s$ for each k-step, are assumed to be input variables, and the discrete nonholonomic flow these equations generate is of the form

$$\begin{array}{rccc}
\widehat{F}_{L_d,\Lambda}: & TQ|_N \times \Lambda \times U^s & \to & TQ|_N \times \Lambda\\
& \left(q_k, v_k, \lambda_k, \{U_k^i\}_{i=1}^s\right) & \mapsto & (q_{k+1}, v_{k+1}, \lambda_{k+1})\,.
\end{array}$$

As we saw in the previous section, if we are going to use this discrete dynamical system as the plant of an optimal control problem, we will need to either solve for λ_{k+1}

and $\{\Lambda_k^i\}_{i=2}^{s-1}$ or impose their variations. This is required in order to derive the correct discrete necessary conditions for optimality. The first option is generally too difficult and involved, leaving us with the second option.

The previous system of equations can be recast as the function

$$\mathcal{F}(x, y) = 0$$

where $x = (q_k, v_k, \lambda_k, U_k^1, ..., U_k^s)$, $y = (q_{k+1}, v_{k+1}, \lambda_{k+1}, \Lambda_k^2, ... \ ..., \Lambda_k^{s-1}, ...)$.

As we are assuming that the problem is regular and compatible, from theorem 5.2.1 we know that it is possible to differentiate the system

$$\frac{\partial \mathcal{F}}{\partial x}\delta x + \frac{\partial \mathcal{F}}{\partial y}\delta y = 0$$

and solve for δy, as $\frac{\partial \mathcal{F}}{\partial y}$ must be invertible, at least in a neighborhood of the solution. Thus,

$$\delta y = -\left(\frac{\partial \mathcal{F}}{\partial y}\right)^{-1} \frac{\partial \mathcal{F}}{\partial x}\delta x \,.$$

This way we get $\{\delta\Lambda_k^i\}_{i=2}^{s}$ in terms of $\delta q_k, \delta v_k, \delta\lambda_k, \{\delta U_k^i\}_{i=1}^{s}$, which is exactly what we needed.

Even if obtaining these variations is easier than solving for the actual variables, inverting $\frac{\partial \mathcal{F}}{\partial y}$ symbolically might be problematic. Nevertheless, it is possible to side-step this problem by deferring this computation to a later stage where only a numerical inversion is necessary. The details for this will not be provided here.

Let us write these relations as

$$\delta\Lambda_k^i = R_k^{q,i}\delta q_k + R_k^{v,i}\delta v_k + R_k^i\delta\lambda_k + \sum_{j=1}^{s} R_k^{U^j,i}\delta U_k^j \,.$$

If we take variations of the discrete extended cost function,

$$\begin{aligned}
&\bar{\mathcal{J}}_d[\bar{c}_d] = \\
&\sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \Bigg[C\left(Q_k^i, V_k^i, U_k^i\right) \\
&+ \left\langle \mathrm{M}_{Q,k}^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij}V_k^j \right\rangle + \left\langle \mu_{q,k+1}, \frac{q_{k+1} - q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle \\
&+ \left\langle \mathrm{M}_{P,k}^i, \frac{D_2L(Q_k^i, V_k^i) - D_2L(q_k, v_k)}{h} - \sum_{j=1}^{s} \hat{a}_{ij}\left[...(Q_k^j, V_k^j, U_k^j, \Lambda_k^j)\right] \right\rangle \\
&+ \left\langle \mu_{p,k+1}, \frac{D_2L(q_{k+1}, v_{k+1}) - D_2L(q_k, v_k)}{h} - \sum_{j=1}^{s} \hat{b}_j\left[...(Q_k^j, V_k^j, U_k^j, \Lambda_k^j)\right] \right\rangle \Bigg] \,,
\end{aligned}$$

then we can add the imposed variations

$$\begin{aligned}
&\left\langle \delta\bar{\mathcal{J}}_d[\bar{c}_d], \delta\bar{c}_d \right\rangle \\
&+ \sum_{k=0}^{N-1}\sum_{i=2}^{s} hb_i \left\langle \mathrm{M}_{\Lambda,k}^i, \delta\Lambda_k^i - R_k^{q,i}\delta q_k - R_k^{v,i}\delta v_k - R_k^i\delta\lambda_k - \sum_{j=1}^{s} R_k^{U^j,i}\delta U_k^j \right\rangle = 0 \,.
\end{aligned}$$

Of course, to close the system we must add the equations

$$\begin{aligned} D_2L(q_k^i, v_k^i) &= D_2L(q_k, v_k) \\ &\quad + h\sum_{j=1}^{s} a_{ij}\left[D_1L(Q_k^j, V_k^j) + f(Q_k^j, V_k^j, U_k^j) + \Lambda_k^j D_2\Phi(Q_k^j, V_k^j)\right] , \\ q_k^i &= Q_k^i, \\ 0 &= \Phi(q_k^i, v_k^i) , \end{aligned}$$

to the resulting ones from the variations.

Example 5.7.2. (Discrete Nonholonomic controlled particle). We have applied the above method with a 3-stage Lobatto method (order 4) to the same model as in example 5.7.1, with the cost function defined in eq.(5.52). Using $N = 25$ steps with total time $T = 5$ and initial and final conditions

$$\begin{aligned} (x_0, y_0, z_0, v_{x,0}, v_{y,0}, v_{z,0}) &= (1, 1, 0, 1, -1/2, 1) , \\ (x_T, y_T, z_T, v_{x,T}, v_{y,T}, v_{z,T}) &= (4, 3, 1, -1/3, 0, -1) . \end{aligned}$$

Also necessary for the method is $\lambda_0 = -1/4$, obtained from $\kappa(y_0, v_{x,0}, v_{y,0})$.

The problem results in a large set of nonlinear equations which must be solved simultaneously, although a shooting method approach is probably possible. In order to solve the problem, we have made use of `fsolve` in MATLAB. The success of the algorithm did not seem to be very dependent on the given initial guess trajectory. A simple straight trajectory not satisfying the nonholonomic constraints from the initial to the final point can be used without problems.

The resulting optimally controlled nonholonomic trajectory can be seen in figs. 5.11 and 5.12.

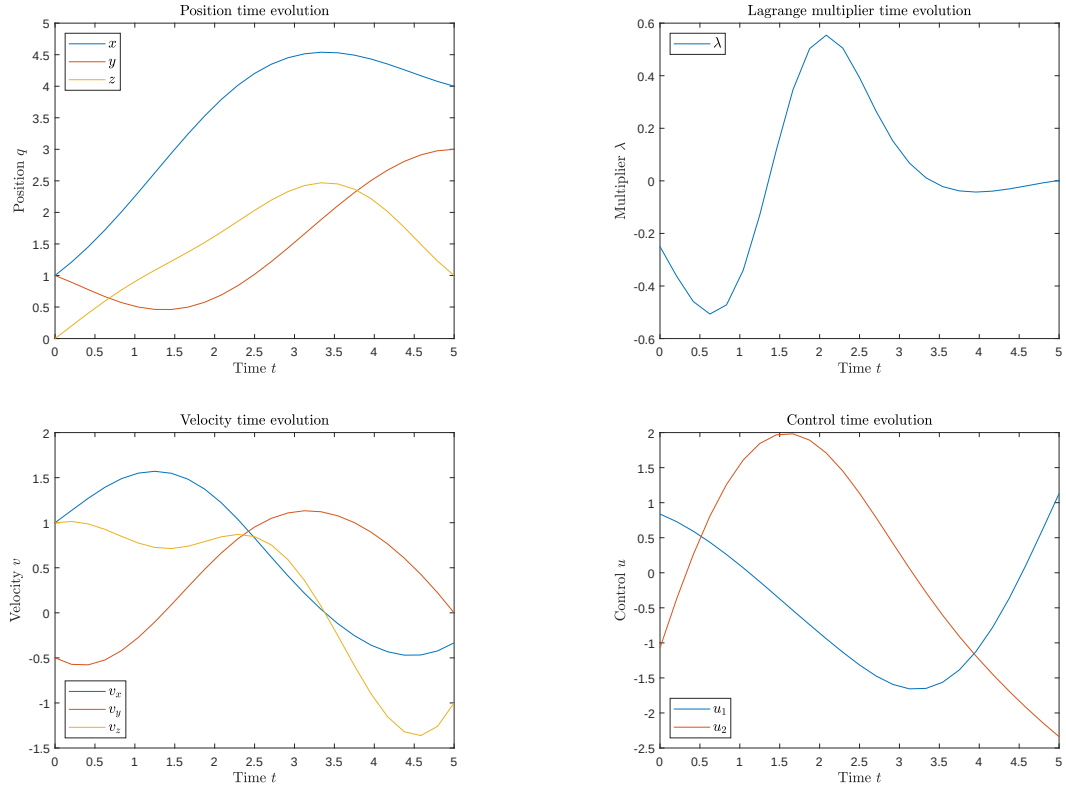


Figure 5.11: Evolution plots of the different magnitudes of interest of the problem: positions, velocities, Lagrange multiplier and controls. By construction, every single step of the evolution satisfies the nonholonomic constraint.

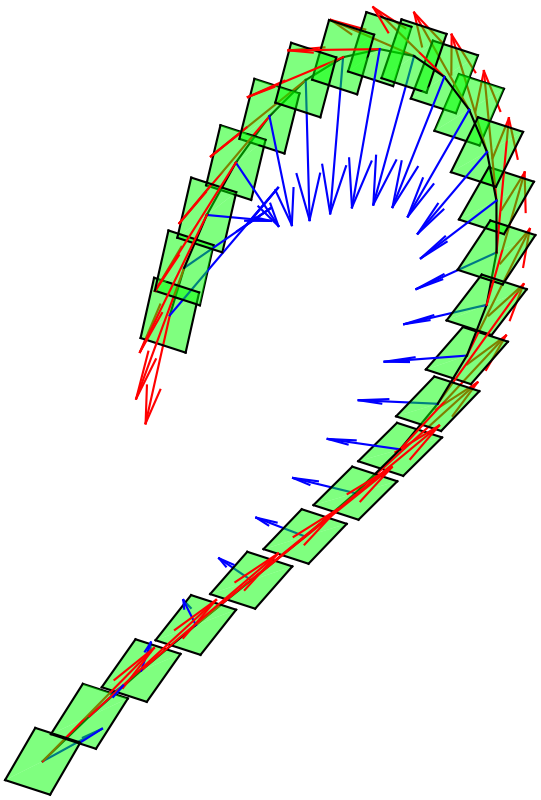


Figure 5.12: Three-dimensional representation of the controlled nonholonomic trajectory. The black line is the trajectory itself. At each step of the trajectory a green plane has been drawn representing the nonholonomic distribution where velocities must lie. The red arrows represent the instantaneous velocity of the particle and the blue arrow represents the control force.

Chapter 6

Conclusions and Future work

In this thesis we have explored the field of geometric mechanics, in particular discrete mechanics. We have focused primarily on its applications to geometric integration on vector spaces and Lie groups. We have studied the cases of systems subject to external forces and nonholonomic systems, two cases where some open problems still remained.

The main contributions of this thesis are the following:

1. We have shown how to construct high-order Lie group integrators from a variational point of view and without resorting to any truncation.

2. We have studied the relation of these methods with the geometry of $T^{(2)}\mathfrak{g}$ and $T^{(2)}G$.

3. For forced systems:

   - Using the technique of duplication of variables we have rigorously deduced the error analysis of forced mechanical systems in terms of previously existing results on variational error.
   - We extended these results to the setting of symmetry reduction, deriving the forced Euler-Poincaré and Lie-Poisson equations variationally.
   - We have elucidated the geometry of the procedure of duplication of variables, which connects with the concept of symplectic and Poisson groupoids.
   - Moreover, we have separately studied the Hamiltonian and Lagrangian formalism and established their mutual relation.

4. We proposed a new geometric integration algorithm for partitioned index 2 DAEs and proved its order.

5. For nonholonomic systems:

   - We have applied the new proposed integrator to the case of nonholonomic mechanics, both on vector spaces and Lie groups, and we have shown how it relates to the holonomic case.
   - We have briefly explored its relation with the nonholonomic Hamilton-Jacobi equation.
   - Using this method we have succesfully posed and shown how to numerically solve nonholonomic optimal control problems.

The research outlined here has been the subject of several papers. [MS18b] was published in Nonlinearity, and [Sat18] and [MS18a] have been submitted to BIT Numerical Mathematics and Journal of Nonlinear Science respectively. Both are pending some corrections on our part.

We carried out further research on related areas during this period which we have not included in this dissertation:

- Geometric integration of time-dependent mechanical systems: The geometry of these systems is naturally cosymplectic and these manifolds can be studied as leaves of a foliation of a higher dimensional symplectic manifold. The leaves themselves can also be foliated into lower dimensional symplectic manifolds. This Russian doll structure has consequences for numerical integration.

- Generation of geometric methods suited for parallel computing through iterative approaches.

- High-order geometric integrators based on collocation for higher order Lagrangian theories, such as splines and elastic models (e.g. Euler's elastica).

- General application of geometric methods to the field of optimal control, from kinematic problems and optimal time problems to discontinuous (bang-bang) controls and tracking problems.

- Shape analysis and its interplay with geometric integrators.

- Spline generation on Lie groups, where $\mathrm{dd}^L\tau$ also appears naturally.

A paper on a geometric approach to tracking control [Nay+19] was submitted to the American Control Conference 2019 and has been accepted.

There are several open research topics left that we hope other researchers and us will be able to pursue:

1. Energy behaviour of forced integrators: We know that the overall behaviour of forced integrators is excellent, and numerical tests seem to show that their energy behaviour is comparable to the free case. We believe that by using the duplication of variables approach we should be able to obtain some results in this direction. One of the main issues is that, due to the way the theory is built, we need to restrict to the identities $\epsilon(Q) \subset Q \times Q$ in order to obtain forced dynamics on Q, and there the free Hamiltonian $\boldsymbol{H}_f : T^*Q \times T^*Q \to \mathbb{R}$ vanishes. Nevertheless, the Hamiltonian itself is not singular there, so perhaps something can be said about the energy of the system in Q.

2. Double bracket dissipation [Blo+96]: An important feature of these systems is the conservation of coisotropic orbits and Casimir functions while displaying energy dissipation. Can the duplication of variables be exploited to construct high-order methods for this particular case of reduced systems and preserve its properties? Can it be used to explain the good behavior of existing methods?

3. Is it possible to use our results of forced integrators to prove the order of our nonholonomic method? We do not know yet how to deal with the Lagrange multipliers satisfactorily.

4. Further research into the nonholonomic Hamilton-Jacobi equation both in the augmented and restricted settings need to be carried out, particularly on existence and correct definition of complete solutions for these systems. This might lead to a better way of constructing and proving the order of nonholonomic integrators.

5. Γ-convergence of the nonholonomic integrator and exploration of pathological cases. The Chaplygin sleigh in particular seems to behave badly with the proposed algorithm. If a non-conservative version of the algorithm is applied (computing $\lambda_{k+1} = \kappa(q_{k+1}, v_{k+1})$ for the following step), the conservative energy behaviour is destroyed but the overall correct behavior of the system is regained. Can we explain why this happens and control it?

6. Study how to apply mixed discretizations to the nonholonomic case. These have already been succesfully applied in the holonomic case [WOL17].

7. High-order nonholonomic Galerkin methods: Right now we do not know how to correctly impose the constraints on inner stages.

8. Application of our ideas for the nonholonomic integrator to field theories as in [Van07], where a Cosserat-type rod was constrained to roll on a flat surface while under torsion. In that paper a method similar to [CM01] was used. It would be a good example of application of both our high-order schemes for nonholonmic systems and our collocation methods for higher order Lagrangian theories in conjunction.

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