Karlsruhe Institute of Technology

Institute of Mechanics

Prof. Dr.-Ing. habil. Peter Betsch
Prof. Dr.-Ing. habil. Thomas Seelig

Master Thesis

A Mixed Variational Framework for the Structure-preserving Integration of Dynamical Systems with Primary and Secondary Constraints

by

Philipp Lothar Kinon, B. Sc.

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Supervisors: Mark Schiebl, M. Sc.
Simeon Schneider, M. Sc.
Examiner: Prof. Dr.-Ing. habil. Peter Betsch

Für dich, Papa.

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Abstract

The present work introduces a novel variational principle for the dynamics of constrained systems. It is inspired by the mixed character of *Livens principle*, unifying Lagrangian and Hamiltonian viewpoints and takes account of both primary and secondary constraints. The emanating equations of motion can be viewed as generalization of the classical *Gear-Gupta-Leimkuhler (GGL) stabilization* and thus justify it in a variational sense. Contrary to the original version, the newly proposed formalism provides a set of differential-algebraic equations with Hamiltonian structure. Furthermore, based on the new framework, this thesis provides two novel structure-preserving integrators: a two-parameter family of symplectic *variational integrators* and an *energy-momentum consistent* integration scheme. Numerical investigations eventually show that the derived integrators exhibit desireable numerical properties and inherit the conservation principles of the time-continuous equations of motion.

Keywords Constrained dynamics · Primary and secondary constraints · Mixed variational principle · GGL stabilization · Symplectic structure · Hamiltonian structure · Structure-preserving time integration

Kurzfassung

Die vorliegende Thesis präsentiert ein neues Variationsprinzip für die Dynamik gebundener Systeme, welches primäre sowie sekundäre Zwangsbedingungen berücksichtigt. Inspiriert vom gemischten *Livens Variationsprinzip* vereint es Lagrangesche und Hamiltonsche Darstellungsweisen. Die entstehenden Bewegungsgleichungen können schließlich als Verallgemeinerung der klassischen *Gear-Gupta-Leimkuhler (GGL) Stabilisierung* angesehen werden, welche somit variationell begründet wird. Im Gegensatz zur ursprünglichen Version haben die neuen Bewegungsgleichungen allerdings Hamiltonsche Struktur. Auf dem Variationsprinzip aufbauend werden folglich zwei neuartige strukturerhaltender Integratoren hergeleitet: eine symplektische Zwei-Parameter-Familie *variationeller Integratoren* und ein *Energy-Momentum-Verfahren*. Mithilfe numerischer Beispiele wird schließlich gezeigt, dass die Integrationsverfahren gewünschte numerische Eigenschaften aufweisen und die Erhaltungsgrößen der zeitkontinuierlichen Bewegungsgleichungen erfassen.

Schlüsselwörter Dynamik gebundener Systeme · Primäre und sekundäre Zwangsbedingungen · Gemischtes Variationsprinzip · GGL Stabilisierung · Symplektische Struktur · Hamiltonsche Struktur · Strukturerhaltende Zeitintegration

Contents

1 Introduction

The desire to describe, understand and predict the motion of dynamical systems has outlasted several centuries until now. From the first ideas of Aristotle (384-322 BC) and Galileo Galilei (1564-1642) over Isaac Newton's *Principia Mathematica* in 1687 and Joseph-Louis Lagrange's *Mécanique Analytique* in 1788 and later contributions such as the foundation of Hamiltonian mechanics by William Hamilton in 1833, our knowledge about dynamical processes has deepened immensely. In the last decades, the main focus has become to derive mathematical tools which solve the equations of motion in an approximative manner. For this purpose, it is firstly essential to describe the given problems with an appropriate set of variables.

Dynamical systems may be formulated in various ways. The well-known Lagrangian and Hamiltonian formalisms both consider descriptive energetic scalars and deploy certain operations on them to generate the system's *equations of motion* (cf. Greenwood [1]). On the one hand, Hamiltonian mechanics formulate a *Hamiltonian* H as a function of independent positions and momenta, which yields the equations of motion after differentiation. On the other hand, Lagrangian formalisms rely on the *Lagrangian* L, which is a function of positions and corresponding velocities. Thus, the dynamics of the system are governed by the variational stationarity of the integral of L over the whole motion, the *action integral*. Consequently, for a system with d degrees of freedom, Lagrange's equations of motion are a set of d second-order *differential equations*, whereas the Hamiltonian equations of motion are obtained as $2d$ first-order differential equations. However, both formalisms can be viewed as two sides of the same coin of analytical mechanics. Both frameworks are equivalent to the classical Newtonian dynamics and have been studied thoroughly (cf. textbooks by Goldstein [2], Holm et al. [3] or Arnold [4]).

Another century later in 1919, G.H. Livens proposed a new formulation [5], which unifies both above-mentioned formalisms by means of independent position, velocity and momentum quantities. This *Livens principle* has been recently taken up by Bou-Rabee [6], [7], Yoshimura et al. [8] and Holm [9] under the name of *Hamilton-Pontryagin principle* due to its close relation to the *Pontryagin principle* from the field of optimal control [10]. Livens principle allows for an advantageous universal description due to its mixed character and is equivalent to both above-mentioned frameworks of analytical dynamics.

In any formalism, which allows for the accumulation of positions and momenta in a so-called *phase space vector*, the equations of motion can be brought into an insightful, yet abstract way (cf. Marsden et al. [11] or Leimkuhler et al. [12]). This Hamiltonian viewpoint facilitates the further analysis of the system's symmetries and correponding conservation principles concerning the *momentum maps* (e.g. Hamiltonian, linear and

angular momentum) and the *symplectic structure*. The rather abstract property of symplecticness induces the conservation of the phase space volume during motion and leads to other invariants as well (cf. Leimkuhler et al. [12]). A very expedient notation of the symplectic structure is provided by the *wedge product* of position and momentum vectors (cf. Leimkuhler et al. [12]).

A large variety of dynamical systems are subject to *constraints*, which reduce the degrees of freedom of the system and impose some constraint function to be satisfied. In those cases, the governing equations can either be described in a set of *minimal coordinates*, which emerge from the knowledge of the system's degrees of freedom or in *redundant coordinates* where no preliminary knowledge is necessary. In the latter situation, the equations of motion emerge as a set of *differential-algebraic equations* (DAEs), which combine both differential equations and algebraic constraint equations. It is to mention that the numerical treatment of DAEs requires some additional effort compared to purely differential equations (cf. Kunkel et al. [13]). However, the presence of constraints does not alter the symmetries of the dynamical systems on the whole. Thus, constrained systems can be shown to be symplectic as well and conserve momentum maps along their solutions (cf. Leimkuhler et al. [12] and Gonzalez [14]). As the constraints have to hold at every point in time (*consistency condition*), so-called *secondary constraints* for the position and velocity quantities are induced.

In a vast majority of dynamical problems, one cannot find an analytical solution. Thus, in recent times, the focus of scientific research has become to derive *numerical integration* methods, which are capable of solving the equations of motion approximately. Therefore, the class of *structure-preserving integrators* seeks to inherit the already named conservation principles of dynamical systems in a discrete sense (cf. monographs such as Hairer et al. [15] or Leimkuhler et al. [12]). The first contributions can be traced back to symplectic methods (see e.g. Vogelaere [16]). In the field of mechanics, research has mainly focussed on the preservation of energy, momentum maps and symplectic structure. However, it can be shown that those target quantities cannot be conserved at once while maintaining a fixed time step size (cf. Zhong et al. [17]). Consequently, structure-preserving integration schemes can be mainly divided into two different groups: *variational integrators* and *energy-momentum integrators*.

Variational integrators approximate the action integral and are typically able to conserve the symplectic structure as well as the system's momentum maps in a discrete sense (cf. Lew et al. [18]). These are consequences of the variational procedure of derivation (cf. Marsden et al. [19]). The main idea to find discrete counterparts of the variational principles goes back to Maeda [20]. Based on this concept, Marsden et al. [19] provided a framework of discrete Lagrangian and Hamiltonian mechanics. Until now, variational integrators have been developed for various applications: For shell structures (cf. Grinspun [21]) and geometrically exact beams (cf. Demoures et al. [22]) as well as for flexible multibody dynamics (cf. Betsch et al. [23]), optimal control (cf. Jiménez et al. [24], Betsch et al. [25]), molecular dynamics (cf. Leyendecker et al. [26]) and also for fluid dynamics (cf. Gawlik et al. [27]). Last but not least, constrained dynamical systems can be solved with appropriate variational integrators as well (see e.g. Leyendecker et al. [28] or Wenger et al. [29]). So far, variational integrators for constrained dynamics predominantly do not

conserve the constraint phase space, i.e. secondary constraints are not satisfied. The present work aims at filling this gap.

Another way to construct structure-preserving integration schemes are the so-called energy-momentum (EM) integrators which originate from works by Greenspan [30], LaBudde et al. [31] and Simo et al. [32]. Later, a systematic approach using discrete gradient operators has been provided by Gonzalez [33] and [34]. As the name suggests, EM schemes conserve energy and momentum in a discrete sense. However, they fail to preserve the symplectic structure of a dynamical system. EM integrators have yet been developed in various research fields such as nonlinear elastodynamics (cf. Simo et al. [35]), finite viscoelasticity (cf. Groß et al. [36]), thermo-elastodynamics (cf. Groß et al. [37]), structural elements (cf. Romero et al. [38] and Pimenta et al. [39] for rods, Leyendecker et al. [40] for geometrically exact beams and Simo et al. [41] and Campello et al. [42] for shells), multibody dynamics (cf. Betsch et al. [43] and [23]), dynamic contact problems (see e.g. Betsch et al. [44]) and quaternion-based rigid body dynamics (cf. Betsch et al. [45]). A comprehensive overview can be found in Betsch [46]. Also constrained dynamical systems can be solved by means of EM integrators. Gonzalez [14] contributed a scheme in 1999 and thus generalized his work from 1996 [33]. Another work dealing with EM schemes for constrained dynamics has been provided by Leyendecker [47]. For a comparison with other approaches such as the Penalty method for constrained Hamiltonian dynamics we refer to Leyendecker et al. [48].

Integration schemes for constrained dynamics typically only account for the constraint on configuration level (*primary constraint*) but not for the secondary constraint and thus have a *differentiation index* of 3. This may lead to numerical instabilities, especially when singular points exist (cf. Yoshimura [49]). By replacing the primary constraints on position level with the secondary velocity-level constraints, DAEs with index 2 are obtained. Thus, the numerical problems can be avoided but violations of the primary constraints are induced (cf. Yoshimura [49]). However, this issue can be alleviated by extending the system of unknowns and coupling the secondary constraints into the equations. The most famous technique, the *Gear-Gupta-Leimkuhler (GGL) stabilization*, traces back to Gear et al. [50] in 1985 and is widely used until today (cf. Brüls et al. [51] and Arnold et al. [52] and [53]). This classical GGL formulation relies on the direct modification of the equations of motion. Yet, this procedure leads to a destruction of the Hamiltonian structure such that most GGL stabilized integration schemes are not symplectic.

To the best of the author's knowledge, numerical integration schemes for constrained dynamics have been formulated either in a Hamiltonian or in a Lagrangian way. Moreover, variational integration schemes have not been yet constructed such that primary and secondary constraints are satisfied at once. Thus, this work tries to fill both gaps by introducing a novel Livens-based variational framework for the integration of dynamical systems accounting for both primary and secondary constraints. Thus, the new framework enables us to justify the commonly used GGL formulation in a variational sense. Contrary to the original version, the newly proposed formalism provides index 2 DAEs with a Hamiltonian structure, which allows us to opt for an EM conserving discretization as well. Moreover, the newly proposed variational principle opens up a plethora of new variational integration schemes with a GGL-based stabilization. A main goal of this

work is therefore to derive both symplectic variational integrators and EM schemes that are capable of satisfying primary and secondary constraints.

The present thesis exclusively deals with spatially discrete systems, i.e. particle systems and discretized rigid body systems. This allows for an application in several fields such as multibody dynamics, molecular dynamics, systems with optimal control and many more. However, most integration schemes derived for those cases have been succesfully applied to spatially continuous systems as well (see above for the application of variational integrators and EM integrators in the respective contexts). This requires the application of spatial discretization technique such as the *Finite Element Method*.

The present work is structured as follows. Chapter 2 covers the basics and fundamentals of Lagrangian and Hamiltonian dynamics for systems without constraints or described in minimal coordinates. Corresponding symmetries and conservation principles are discussed as well as the mixed Livens principle. In Sec. 2.4 we also give a short introduction into the concept of variational integrators and time-discrete conservation principles. Subsequently, Chapter 3 gives an overview of holonomic constraints. It will be shown how variational principles for dynamical systems can account for constraints and how the conservation laws are described in that case. Moreover, the concept of differentiation indices for DAEs are explained and previously derived integration schemes for constrained systems are demonstrated. The chapter concludes with a description of rigid body dynamics based on a director formulation, which allows for a DAE representation of the equations of motion (see e.g. Betsch et al. [54] or [55] or [56] or Krenk [57]). In Chapter 4 we will introduce the novel variational principle together with the emanating equations of motion and pertinent conservation principles. Subsequently, we will construct novel integration schemes. First, we will straightforwardly discretize the novel functional in analogy to a constrained symplectic Euler scheme. Next, we will apply an ansatz, already used in optimal control by Betsch et al. [25], which makes use of auxiliary variables. Lastly, an EM scheme with secondary constraints as an extension of the work by Gonzalez [14] will be covered in detail. All the integration schemes will be analyzed by means of numerical examples in order to investigate the respective numerical properties. Eventually, a summary of the thesis and concluding remarks as well as an outlook on further research ideas will be given in Chapter 5.

The appendix gives additional information on some issues discussed in the main part of this thesis. Appendix A provides an overview of the mathematical notation used throughout this work and crucial properties of the wedge product. Appendix B covers a detailled proof, that the family of variational integrators derived in Sec. 4.3 is symplectic. Appendix C shows newly derived integration schemes that have been mentioned in the main part and will provide detailed governing equations and a numerical analysis. Appendix C.2 in particular shows a modified one-parameter method evolving from the symplectic theta method which can be linked to the EM scheme from Sec. 4.4.

The numerical computations throughout this work have been performed with the *metis* code, which has been implemented by the author for the purpose of this thesis. It is freely available at [58].

2 Dynamics of Discrete Systems

This chapter covers the basics and fundamentals of discrete dynamical systems, which are necessary to understand the topics throughout this thesis. Section 2.1 deals with the variational principles and corresponding equations of motion of a dynamical system. This allows for a further analysis of underlying symmetries and conservation laws in Section 2.2. In Section 2.3 the focus is set on the symplectic structure of Hamiltonian systems. For the numerical integration, the concept of variational integrators becomes crucial during this thesis. Therefore, we provide the basics of variational integrators in Section 2.4.

2.1 Variational Principles and Governing Equations

Throughout this section, several variational frameworks for the analysis of dynamical systems are introduced. We start with the most commonly known framework of Lagrangian dynamics in Section 2.1.1. In Section 2.1.2 the Hamiltonian of a dynamic system will be introduced and the Hamiltonian equations of motion will be derived. Finally, a mixed variational principle called *Livens principle* based on the usage of Lagrange multipliers will be covered in Section 2.1.3.

2.1.1 Lagrangian Dynamics

This introductory chapter mainly follows along the introduction of Lagrangian mechanics provided by Lew et al. [18]. The fundamentals of manifolds and geometric mechanics can be found in various monographs, e.g. by Holm et al. [3] or Arnold [4].

Let the space of all positions $\mathbf{q}(t)$ of a mechanical system with d degrees of freedom be denoted as the *configuration manifold* $\mathcal{Q} \subset \mathbb{R}^d$. Thus, for any point along the trajectory of a system the velocities $\dot{\mathbf{q}}$ are given by the temporal derivative (A.1) of $\mathbf{q}$ and belong to the *tangent space* $\mathcal{T}_{\mathbf{q}}\mathcal{Q}$. For a depiction of the tangent space see Fig. 2.1. Furthermore, the *tangent bundle* $\mathcal{T}\mathcal{Q}$ is the union of all tangent spaces to $\mathcal{Q}$, viz.

$$\mathcal{T}\mathcal{Q} = \bigcup_{\mathbf{q}\in\mathcal{Q}} \mathcal{T}_{\mathbf{q}}\mathcal{Q} \,. \tag{2.1}$$

Accordingly, all pairs of positions $\mathbf{q} \in \mathcal{Q}$ and velocities $\dot{\mathbf{q}} \in \mathcal{T}_{\mathbf{q}}\mathcal{Q}$ belong to the tangent bundle, meaning $(\mathbf{q}(t), \dot{\mathbf{q}}(t)) \in \mathcal{T}\mathcal{Q}$.

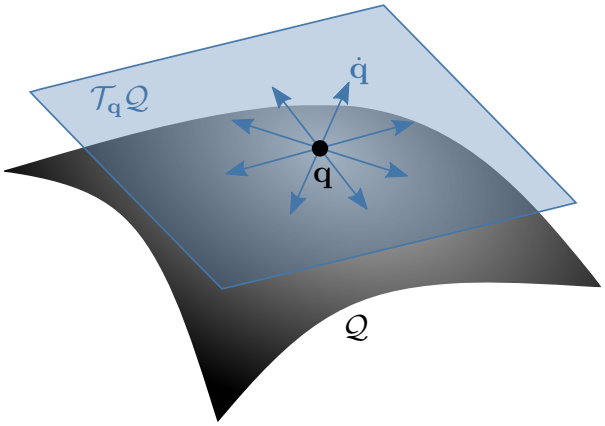

Figure 2.1: Configuration manifold $\mathcal{Q}$ and tangent space $\mathcal{T}_\mathbf{q}\mathcal{Q}$

In the framework of Lagrangian mechanics it is crucial to define the scalar-valued *Lagrangian* $L : \mathcal{TQ} \to \mathbb{R}$ for *natural* and *autonomous* mechanical systems as

$$L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}} \cdot \mathbf{M}(\mathbf{q})\dot{\mathbf{q}} - V(\mathbf{q}) \tag{2.2}$$

with the potential energy function $V : \mathcal{Q} \to \mathbb{R}$ and the invertible and symmetric mass matrix $\mathbf{M} : \mathcal{Q} \to \mathbb{R}^{d\times d}$, which may depend on the configuration of the system. Being autonomous refers to the fact that the Lagrangian is only implicitly time-dependent. So-called natural systems allow for the representation in which the Lagrangian is equal to the difference between kinetic and potential energy (cf. Arnold [4]). The system's equations of motion can be derived by making use of *Hamilton's principle of stationary action*, which states that the motion of a mechanical system over the time interval $t \in [0, T]$ is given by the extremum of the *action integral*

$$S(\mathbf{q}) = \int_0^T L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\,\mathrm{d}t\ . \tag{2.3}$$

Thus, a path $\mathbf{q}(t)$, as depicted in Fig. 2.2, is a solution of the equations of motion if and only if it represents a stationarity point of the functional S. This stationarity can be expressed in terms of the *first variation* (A.8) of the above-mentioned functional, which is given by

$$\delta S(\mathbf{q}) = \mathrm{D}S(\mathbf{q}) \cdot \delta\mathbf{q} \tag{2.4}$$

with the variations $\delta\mathbf{q} \in \mathcal{T}_\mathbf{q}\mathcal{Q}$. The gradient operator $\mathrm{D}(\bullet)$ is defined in (A.2). Hence, Hamilton's principle reads

$$\delta S(\mathbf{q}) = \int_0^T \delta L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\mathrm{d}t = 0\ , \tag{2.5}$$

where we can take the variation into the integral since temporal and spatial operators do not interfere here. It is essential to state that admissible variations of the configuration

are arbitrary but need to satisfy the endpoint conditions

$$\delta\mathbf{q}(t=0) = \delta\mathbf{q}(t=T) = \mathbf{0} \ . \tag{2.6}$$

The procedure of advancing from the variational principle (2.5) to the resulting equations of motion is based on the execution of the first variation of L, integration by parts and making use of the endpoint conditions (2.6). For further details see Holm et al. [3]. In view of the arbitrariness of the variations one eventually arrives at

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D}_2 L(\mathbf{q},\dot{\mathbf{q}}) - \mathrm{D}_1 L(\mathbf{q},\dot{\mathbf{q}}) = \mathbf{0} \ , \tag{2.7}$$

which is commonly known as *Lagrange's equations of the second kind* and where $\mathrm{D}_i(\bullet)$ denotes the partial derivative (A.3). The last equations are referred to as *Euler-Lagrange equations* (EL equations) of the system and represent the governing equations of motion, which are in agreement with Newton's laws. Throughout this thesis we consider dynamical systems with a constant, invertible and symmetric mass matrix $\mathbf{M} \in \mathbb{R}^{d\times d}$ such that the system's Langrangian is given by

$$L(\mathbf{q},\dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}}\cdot\mathbf{M}\dot{\mathbf{q}} - V(\mathbf{q}) \ . \tag{2.8}$$

Thus, Lagrange's equations of the second kind yield

$$\mathbf{M}\ddot{\mathbf{q}} = -\mathrm{D}V(\mathbf{q}) \ , \tag{2.9}$$

where we have "mass times acceleration" on the left hand side and all conservative forces emanating from a potential on the right hand side.

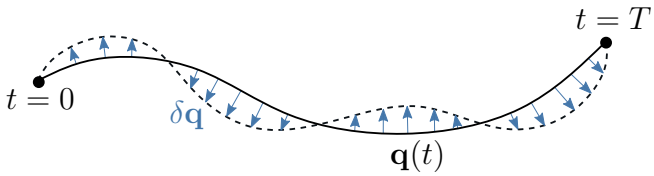

Figure 2.2: Variations along path $\mathbf{q}(t)$ with fixed endpoints

2.1.2 Hamiltonian Dynamics

The fundamental concepts of Hamiltonian dynamics, which are dealt with in this section, are mainly following along Lew et al. [18] but can also found in various textbooks such as Holm et al. [3].

By defining the so-called *conjugate momenta* as

$$\mathbf{p} = \mathrm{D}_2 L(\mathbf{q},\dot{\mathbf{q}}) \ , \tag{2.10}$$

it is possible to switch from velocities to momenta as the second variable. Thus, a map $F_L : \mathcal{TQ} \to \mathcal{P}$ is introduced as the *Legendre transformation*. Therefore, Hamiltonian mechanics consider a set of variables $(\mathbf{q}, \mathbf{p}) \in \mathcal{P}$, where $\mathcal{P} \subset \mathbb{R}^{2d}$ denotes the so-called *phase space*. Note that the phase space is equivalent to the *cotangent bundle* $\mathcal{T}^*\mathcal{Q}$. Consequently, the map is given by

$$(\mathbf{q}, \mathbf{p}) = F_L(\mathbf{q}, \dot{\mathbf{q}}) \tag{2.11}$$

with the corresponding *fiber derivative* of L defined in (2.10). Lew et al. [18] state that F_L is bijective and thus invertible "for typical mechanical systems [...] because the Lagrangian is strictly convex in $\dot{\mathbf{q}}$ for each $\mathbf{q}$". This is verified due to the structure of (2.2). Therefore, the inverse map F_L^{-1} is defined for every $\mathbf{p} \in \mathbb{R}^d$ such that

$$(\mathbf{q}, \dot{\mathbf{q}}) = F_L^{-1}(\mathbf{q}, \mathbf{p}) \ . \tag{2.12}$$

Eventually, the *Hamiltonian* $H : \mathcal{P} \to \mathbb{R}$ of a system is defined by

$$H(\mathbf{q}, \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p}) - L(\mathbf{q}, \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p})) \ , \tag{2.13}$$

where the velocities are expressed as a function of $\mathbf{q}$ and $\mathbf{p}$ by (2.12). The Hamiltonian equations of motion can be derived by taking the partial derivatives of H with respect to both independent variables, such that

$$\dot{\mathbf{q}} = +\mathrm{D}_2 H(\mathbf{q}, \mathbf{p}) \ , \tag{2.14a}$$
$$\dot{\mathbf{p}} = -\mathrm{D}_1 H(\mathbf{q}, \mathbf{p}) \ . \tag{2.14b}$$

By taking account of the Lagrangian of autonomous and natural systems given in (2.2) and assuming a constant mass matrix, we obtain

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2} \mathbf{p} \cdot \mathbf{M}^{-1} \mathbf{p} + V(\mathbf{q}) \ . \tag{2.15}$$

Therefore, the Hamiltonian represents the total energy of a closed dynamical system. Eventually, the equations of motion in that case occur in the form

$$\dot{\mathbf{q}} = \mathbf{M}^{-1} \mathbf{p} \ , \tag{2.16a}$$
$$\dot{\mathbf{p}} = -\mathrm{D} V(\mathbf{q}) \ . \tag{2.16b}$$

It is possible (cf. Holm et al. [3]) to proof that the Hamiltonian H is a conserved quantity along trajectories of autonomous dynamical systems, i.e. $H(\mathbf{q}(t), \mathbf{p}(t)$ is constant for any solution of (2.14). For the Hamiltonian formulation this can be easily written as

$$\begin{aligned} \dot{H}(\mathbf{q}, \mathbf{p}) &= \mathrm{D}_1 H(\mathbf{q}, \mathbf{p}) \cdot \dot{\mathbf{q}} + D_2 H(\mathbf{q}, \mathbf{p}) \cdot \dot{\mathbf{p}} \\ &= \mathrm{D}_1 H(\mathbf{q}, \mathbf{p}) \cdot D_2 H(\mathbf{q}, \mathbf{p}) + D_2 H(\mathbf{q}, \mathbf{p}) \cdot (-D_1 H(\mathbf{q}, \mathbf{p})) = 0 \ , \end{aligned} \tag{2.17}$$

but applies to Lagrangian or other formulations in the same way. In the last equation the canonical Hamiltonian equations of motion (2.14a) and (2.14b) have been taken into account.

2.1.3 Livens Principle

From Hamilton's principle one can proceed by allowing the velocities to be independent variables $\mathbf{v} \in \mathbb{R}^d$. Therefore we have to enforce the kinematic relation $\dot{\mathbf{q}} = \mathbf{v}$ by means of a Lagrange multiplier $\mathbf{p} \in \mathbb{R}^d$. The evolving functional reads

$$\tilde{S}(\mathbf{q}, \mathbf{v}, \mathbf{p}) = \int_0^T \left[L(\mathbf{q}, \mathbf{v}) + \mathbf{p} \cdot (\dot{\mathbf{q}} - \mathbf{v}) \right] \mathrm{d}t \ , \tag{2.18}$$

which was firstly termed *Livens principle* (cf. Sec. 26.2 in Pars [59]) after G.H. Livens who proposed this functional for the first time (cf. Livens [5]). More recently, Bou-Rabee et al. [6], [7] and Yoshimura et al. [8] coined the name *Hamilton-Pontryagin principle* for this functional due to its close relation to the classical *Pontryagin principle* from the field of optimal control (cf. Pontryagin[1] et al. [10]). Due to its mixed character with three independent fields $(\mathbf{q}, \mathbf{v}, \mathbf{p})$, it resembles the *Hu-Washizu principle* from the area of elasticity theory (cf. Marsden et al. [60]). Henceforth, the variational principle based on (2.18) shall be referred to as Livens principle.

The Livens principle unifies the Lagrangian and Hamiltonian viewpoint on mechanics and automatically accounts for the Legendre transformation as well as the emerging equations of motion. By stating the stationarity condition

$$\delta \tilde{S}(\mathbf{q}, \mathbf{v}, \mathbf{p}) = \int_0^T \delta \left[L(\mathbf{q}, \mathbf{v}) + \mathbf{p} \cdot (\dot{\mathbf{q}} - \mathbf{v}) \right] \mathrm{d}t = 0 \tag{2.19}$$

and executing the variations with respect to every independent variable, we obtain the three equations of motion

$$\dot{\mathbf{q}} = \mathbf{v} \ , \tag{2.20a}$$
$$\dot{\mathbf{p}} = \mathrm{D}_1 L(\mathbf{q}, \mathbf{v}) \ , \tag{2.20b}$$
$$\mathbf{p} = \mathrm{D}_2 L(\mathbf{q}, \mathbf{v}) \ . \tag{2.20c}$$

Note that in (2.20c) the multiplier $\mathbf{p}$, which represents momentum variables, directly emanates from the principle. Within the framework of Hamiltonian dynamics momentum variables had to be defined a priori in (2.10) or emerged from the Legendre transformation as a fiber derivative of $L(\mathbf{q}, \dot{\mathbf{q}})$. Moreover, it can be seen that after reinserting (2.20b) into (2.20c) and making use of (2.20a), Livens principle traces back to the Lagrangian equations of the second kind (2.7).

As for example shown by Yoshimura et al. [8], the principle can also be written slightly different. By introducing a generalized energy quantity

$$E(\mathbf{q}, \mathbf{v}, \mathbf{p}) = \mathbf{p} \cdot \mathbf{v} - L(\mathbf{q}, \mathbf{v}) \ , \tag{2.21}$$

[1] During his lifetime the mathematician Lev Pontryagin was accused of antisemitism multiple times. The author of this thesis heavily refuses any type of discrimination - antisemitism in particular. Scientific achievements do never excuse any discriminating statements or behavior.

the current variational principle takes the form

$$\delta \int_0^T \left[\mathbf{p} \cdot \dot{\mathbf{q}} - E(\mathbf{q}, \mathbf{v}, \mathbf{p}) \right] \mathrm{d}t = 0 \ . \tag{2.22}$$

Making use of (2.20c), we can solve for the velocities $\mathbf{v}$ as a function of the configuration $\mathbf{q}$ and conjugate momenta $\mathbf{p}$, respectively, viz.

$$\mathbf{v} = \tilde{\mathbf{v}}(\mathbf{q}, \mathbf{p}) \ . \tag{2.23}$$

Thus, it is possible to eliminate the velocity variables such that the generalized energy becomes the Hamiltonian, which has been defined in (2.13), reading

$$H(\mathbf{q}, \mathbf{p}) = E(\mathbf{q}, \tilde{\mathbf{v}}(\mathbf{q}, \mathbf{p}), \mathbf{p}) \ . \tag{2.24}$$

Eventually, the two-field variational principle

$$\delta \int_0^T \left[\mathbf{p} \cdot \dot{\mathbf{q}} - H(\mathbf{q}, \mathbf{p}) \right] \mathrm{d}t = 0 \tag{2.25}$$

remains. It is sometimes referred to as *modified Hamilton's principle* (e.g. Sec. 8-5 in Goldstein [2]), because the emerging EL equations directly appear in the form of the canonical Hamiltonian equations (2.14).

2.2 Symmetries and Conservation Laws

Based on the fundamental formulations for dynamical systems shown in the previous section, the underlying symmetries and conservation laws will be analyzed in further detail in this section. First, the equations of motion of Hamiltonian systems will be recast in a more abstract but insightful way in Section 2.2.1. In Section 2.2.2 aspects such as first integrals and G-invariance will be covered. Towards the end of this section, the concept of momentum maps will be introduced in Section 2.2.3 to describe the conservation of total energy, linear momentum and angular momentum in Hamiltonian dynamics.

2.2.1 Abstract Hamiltonian Equations

This section is following along the works by Gonzalez [33] and Leyendecker [47].

It is quite convenient to accumulate the unknowns $(\mathbf{q}, \mathbf{p})$ of Hamiltonian dynamics in a column vector to define the phase space variable $\mathbf{z} \in \mathcal{P} \subset \mathbb{R}^{2d}$

$$\mathbf{z} = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix} \tag{2.26}$$

such that the Hamiltonian equations of motion (2.14a) and (2.14b) can be recast as

$$\dot{\mathbf{z}} = \Omega_z(\mathrm{D}H(\mathbf{z})) = \mathbb{J}\,\mathrm{D}H(\mathbf{z}) \tag{2.27}$$

with $\Omega_z : \mathcal{P} \to \mathbb{R}^{2d}$ being the symplectic mapping in the sense that $\Omega_z(\mathbf{z}) = \mathbb{J}\mathbf{z}$. The *canonical structure matrix* $\mathbb{J} \in \mathbb{R}^{2d\times 2d}$ is used. For natural systems with the standard Hamiltonian (2.15) it reads

$$\mathbb{J} = \begin{bmatrix} \mathbf{0}_{d\times d} & \mathbf{I}_{d\times d} \\ -\mathbf{I}_{d\times d} & \mathbf{0}_{d\times d} \end{bmatrix} , \tag{2.28}$$

where $\mathbf{I}_{d\times d} \in \mathbb{R}^{d\times d}$ denotes the $d \times d$ identity matrix. According to Leimkuhler et al. [12] Hamiltonian systems "can be generalized in various ways without altering the discussion of their geometric properties in any essential way." Thus, $\mathbb{J}$ can be any invertible and constant matrix satisfying the condition of skew-symmetry

$$\mathbb{J}^{\mathrm{T}} = -\mathbb{J} . \tag{2.29}$$

However, the terminology of "canonical" structure matrix only applies to "even dimensional Euclidean spaces" with the definition in (2.28). Throughout this thesis, we only consider typical mechanical systems with a canonical structure, such that this assumption is valid. Moreover, to any smooth Hamiltonian $H : \mathcal{P} \to \mathbb{R}$ where the phase space is an open subset of $\mathbb{R}^{2d}$ a corresponding associated *Hamiltonian vector field* $\mathbf{X}_{\mathrm{H}} : \mathcal{P} \to \mathbb{R}^{2d}$ is defined by

$$\mathbf{X}_H(\mathbf{z}) = \Omega_z(\mathrm{D}H(\mathbf{z})) \tag{2.30}$$

such that the Hamiltonian equations of motion can be briefly rewritten as

$$\dot{\mathbf{z}} = \mathbf{X}_H(\mathbf{z}) . \tag{2.31}$$

2.2.2 First Integrals and G-Invariance

It is now possible to define a *first integral* of the system $(\mathcal{P}, \Omega_z, H)$, meaning a function $f : \mathcal{P} \to \mathbb{R}$, which is constant along solutions of (2.31), viz.

$$f(\mathbf{z}(t)) = f(\mathbf{z}(0)) , \qquad \forall\, t . \tag{2.32}$$

Consequently, from the vanishing time-derivative of f we can deduce the *orthogonality condition* for Hamiltonian systems

$$\dot{f} = \mathrm{D}f(\mathbf{z}) \cdot \mathbf{X}_{\mathrm{H}}(\mathbf{z}) = 0 , \qquad \forall\, \mathbf{z} \in \mathcal{P} , \tag{2.33}$$

where (2.31) has been used. It is straightforward to show that the Hamiltonian itself is a first integral by plugging in H as the function f such that we arrive at

$$\dot{H} = \mathrm{D}H(\mathbf{z}) \cdot \mathbf{X}_{\mathrm{H}}(\mathbf{z}) = \mathrm{D}H(\mathbf{z}) \cdot \mathbb{J}\mathrm{D}H(\mathbf{z}) , \tag{2.34}$$

where (2.30) has been taken into account. Since the symplectic matrix is skew-symmetric (2.29), some tensor algebra yields

$$\mathrm{D}H(\mathbf{z}) \cdot \mathbb{J}\mathrm{D}H(\mathbf{z}) = -\mathrm{D}H(\mathbf{z}) \cdot \mathbb{J}\mathrm{D}H(\mathbf{z}) \ , \tag{2.35}$$

which vanishes identically such that we have proven $\dot{H} = 0$. Note that this has already been shown in (2.17) for canonical systems with the canonical structure matrix given in (2.28).

Let $\mathcal{G}$ denote a Lie-Group with a symplectic action on the phase space $\mathbf{\Phi} : \mathcal{G} \times \mathcal{P} \to \mathcal{P}$ satisfying

$$\mathbf{\Phi}(\mathbf{g}(0), \mathbf{z}) = \mathbf{z} \ , \tag{2.36}$$

where $\mathbf{g} = \mathbf{g}(\alpha) = \exp(\alpha\boldsymbol{\xi})$ represents a family of α-parameterized elements of $\mathcal{G}$. Note that (2.36) induces $\mathbf{g}(\alpha = 0) = \mathbf{I}$, $\exp(\bullet)$ denotes the exponential map on $\mathcal{G}$ and $\boldsymbol{\xi}$ represents a vector belonging to $\mathcal{T}\mathcal{G}$. If the function f remains invariant under that action, meaning

$$f(\mathbf{\Phi}(\mathbf{g}, \mathbf{z})) = f(\mathbf{z}) \ , \qquad \forall \mathbf{g} \in \mathcal{G} \ , \tag{2.37}$$

then the function is called *G-invariant* and we term the system $(\mathcal{P}, \Omega_z, \mathcal{G}, f)$ a Hamiltonian system with *symmetry*. The so-called *infinitesimal generator* $\boldsymbol{\xi}_P$ of the action corresponding to certain $\boldsymbol{\xi}$ is defined by the relation

$$\boldsymbol{\xi}_P(\mathbf{z}) = \frac{\mathrm{d}}{\mathrm{d}\alpha}\mathbf{\Phi}(\exp(\alpha\boldsymbol{\xi}), \mathbf{z})\Big|_{\alpha=0} = \begin{bmatrix} \mathbf{v}_{\boldsymbol{\xi}} \\ \mathbf{w}_{\boldsymbol{\xi}} \end{bmatrix} \ . \tag{2.38}$$

It is an important property of some Hamiltonian systems, that the Hamiltonian H itself is G-invariant, such that we may consider (2.37) applied to the Hamiltonian. Taking into account the definition above for $\boldsymbol{\xi}_p$, we obtain an orthogonality condition between the infinitesimal generator and the gradient of the Hamiltonian, viz.

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}H(\mathbf{\Phi}(\mathbf{g}(\alpha), \mathbf{z}))\Big|_{\alpha=0} = \mathrm{D}H(\mathbf{z}) \cdot \boldsymbol{\xi}_p = 0 \ . \tag{2.39}$$

2.2.3 Momentum Maps

Furthermore, an at most quadratic *momentum map* $\mathbf{J} : \mathcal{P} \to \mathcal{T}^*\mathcal{G}$ for the action of $\mathcal{G}$ on $\mathcal{P}$ can be defined by

$$\mathrm{D}J_{\boldsymbol{\xi}}(\mathbf{z}) = \mathbb{J}^{-1}\boldsymbol{\xi}_P(\mathbf{z}) \tag{2.40}$$

with $J_{\boldsymbol{\xi}}$ denoting the projection of $\mathbf{J}$ along $\boldsymbol{\xi}$ such that $J_{\boldsymbol{\xi}}(\mathbf{z}) = \mathbf{J}(\mathbf{z}) \cdot \boldsymbol{\xi}$. This momentum map is a first integral of the equations of motion (2.31), which can be shown by (2.30),

(2.31), (2.40) and the skew-symmetry of $\mathbb{J}$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t} J_{\boldsymbol{\xi}}(\mathbf{z}) = \mathrm{D}J_{\boldsymbol{\xi}}(\mathbf{z}) \cdot \mathbf{X}_{\mathrm{H}}(\mathbf{z}) = \mathrm{D}H(\mathbf{z}) \cdot \mathbb{J}^{\mathrm{T}} \mathbb{J}^{-1} \boldsymbol{\xi}_P(\mathbf{z}) = -\mathrm{D}H(\mathbf{z}) \cdot \boldsymbol{\xi}_P(\mathbf{z}) \ . \tag{2.41}$$

Eventually, making use of (2.39) yields

$$\dot{J}_{\boldsymbol{\xi}} = 0 \ . \tag{2.42}$$

Provided this concept, one can assume some form of the action $\boldsymbol{\Phi}$ and therefore show that the Hamiltonian remains invariant under that action. Consequently, it is possible to derive corresponding momentum maps, which are at most quadratic. This is a direct consequence of *Noether's theorem*, which states that the presence of a symmetry leads to the conservation of a quantity along solutions of the equations of motion. The following three principles can be shown:

Conservation of total energy

Interpreting the flow of the Hamiltonian vector field $\mathbf{X}_{\mathrm{H}}$ as a flow $\boldsymbol{\Phi}$, assuming $\mathcal{G} = \mathbb{R}$, one can show that $\boldsymbol{\xi}_P = \mathbf{X}_H(\mathbf{z})\xi$ and thus the momentum map equals the Hamiltonian itself

$$J(\mathbf{z}) = H(\mathbf{z}) \ . \tag{2.43}$$

This is a general property of Hamiltonian systems with autonomous Hamiltonian H, but can be proven in this framework as well. It becomes also evident when comparing the definition of the momentum map (2.40) and the Hamiltonian vector field (2.30).

Conservation of linear momentum

Given a translatory action

$$\boldsymbol{\Phi}(\mathbf{g}(\alpha), \mathbf{z}) = \begin{bmatrix} \mathbf{q} + \alpha \boldsymbol{\xi} \\ \mathbf{p} \end{bmatrix} \tag{2.44}$$

such that $\mathcal{G} = \mathbb{R}^d$, the invariance of the Hamiltonian with respect to translations can be shown. Property (2.36) can be easily verified. From the definition of the infinitesimal generator (2.38) one obtains $\boldsymbol{\xi}_P = [\boldsymbol{\xi} \, , \, \mathbf{0}]^{\mathrm{T}}$. Making use of the definition of the momentum maps (2.40) yields

$$\begin{bmatrix} +\mathrm{D}_{\mathbf{p}} J_{\boldsymbol{\xi}} \\ -\mathrm{D}_{\mathbf{q}} J_{\boldsymbol{\xi}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\xi} \\ \mathbf{0} \end{bmatrix} \tag{2.45}$$

such that, eventually, $J_{\boldsymbol{\xi}} = \mathbf{p} \cdot \boldsymbol{\xi}$. Note that $\mathrm{D}_{\mathbf{q}}(\bullet)$ and $\mathrm{D}_{\mathbf{p}}(\bullet)$ denote the partial derivatives (A.3) with respect to $\mathbf{q}$ and $\mathbf{p}$, respectively. The momentum map corresponding to

translatory invariance thus represents the linear momentum

$$\mathbf{J}(\mathbf{z}) = \mathbf{p} \ . \tag{2.46}$$

Conservation of angular momentum

Let $\mathcal{G} = SO(3)$ be the group of proper rotations such that its action represents a 3D rotation expressed with an orthonormal matrix $\mathbf{R} \in \mathbb{R}^{3\times3}$ satisfying $\mathbf{R}^{\mathrm{T}} = \mathbf{R}^{-1}$ and $\det(\mathbf{R}) = +1$ such that single elements of the phase space $(\mathbf{q}^{(i)}, \mathbf{p}^{(i)})$ are subject to the action

$$\mathbf{\Phi}(\mathbf{R}, \mathbf{z}^{(i)}) = \begin{bmatrix} \mathbf{R}(\alpha)\mathbf{q}^{(i)} \\ \mathbf{R}(\alpha)\mathbf{p}^{(i)} \end{bmatrix} \ . \tag{2.47}$$

Thus, $\boldsymbol{\xi}$ denotes the axis of rotation and $\mathbf{R}(\alpha) = \exp(\alpha\hat{\boldsymbol{\xi}})$ characterizes the rotation under which the Hamiltonian is assumed to be invariant. Accordingly, we obtain

$$\mathbf{R}(\alpha = 0) = \mathbf{I} \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}\alpha}\mathbf{R}(\alpha)\Big|_{\alpha=0} = \hat{\boldsymbol{\xi}} \ , \tag{2.48}$$

where $\hat{\boldsymbol{\xi}}$ denotes a skew-symmetric matrix, which can be used for the notation of infinitesimal rotations $\boldsymbol{\xi} \times \mathbf{q}^{(i)} = \hat{\boldsymbol{\xi}}\mathbf{q}^{(i)}$. Consequently, the infinitesimal generator (2.38) is given by

$$\boldsymbol{\xi}_P = \begin{bmatrix} \boldsymbol{\xi} \times \mathbf{q}^{(i)} \\ \boldsymbol{\xi} \times \mathbf{p}^{(i)} \end{bmatrix} \ . \tag{2.49}$$

Accordingly, the momentum map can be gained from integration as $J_{\boldsymbol{\xi}} = (\mathbf{q}^{(i)} \times \mathbf{p}^{(i)}) \cdot \boldsymbol{\xi}$ and the corresponding momentum map denotes the angular momentum

$$\mathbf{J}(\mathbf{z}^{(i)}) = \mathbf{q}^{(i)} \times \mathbf{p}^{(i)} \equiv \mathbf{L}(\mathbf{z}^{(i)}) \ . \tag{2.50}$$

If the generalized phase space coordinate describes n_b bodies in the three dimensional space then the corresponding momentum map is simply the sum of all contributions

$$\mathbf{J}(\mathbf{z}) = \sum_{i=1}^{n_b} \mathbf{q}^{(i)} \times \mathbf{p}^{(i)} \ . \tag{2.51}$$

In particular, if the system is subject to potential forces $\mathbf{f}$, the conservation of linear and angular momentum applies to translations orthogonal to that direction and rotations about the direction of $\mathbf{f}$. In the following a small example will illustrate this case.

Example: Particle Subject to Gravitation

Consider a particle with the position $\mathbf{q} \in \mathbb{R}^3$ and conjugate momentum $\mathbf{p} \in \mathbb{R}^3$, which is subject to gravitation acting in the negative $\mathbf{e}_3$-direction. The Hamiltonian of the

particle with total mass m thus reads

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2} m\, \mathbf{p}\cdot\mathbf{p} + m\, g\, \mathbf{e}_3 \cdot \mathbf{q}\ , \tag{2.52}$$

where g denotes the acceleration due to gravity. We can firstly analyze the rotational symmetry. Assuming a rotational action according to (2.47), we find

$$H(\Phi(\mathbf{R}_3,\mathbf{z})) = \frac{1}{2} m\, (\mathbf{R}_3\mathbf{p})\cdot(\mathbf{R}_3\mathbf{p}) + m\, g\, \mathbf{e}_3 \cdot \mathbf{R}_3\mathbf{q} \tag{2.53}$$

with $\mathbf{R}_3(\alpha) = \exp(\alpha\hat{\boldsymbol{\xi}}) \in SO(3)$ prescribing a rotation about the $\mathbf{e}_3$-axis corresponding to $\boldsymbol{\xi} = \mathbf{e}_3$. Consequently, we obtain

$$\begin{aligned} H(\Phi(\mathbf{R}_3,\mathbf{z})) &= \frac{1}{2} m\, \mathbf{p}\cdot\mathbf{R}_3^{\mathrm{T}}\mathbf{R}_3\mathbf{p} + m\, g\, (\mathbf{R}_3^{\mathrm{T}}\mathbf{e}_3)\cdot\mathbf{q} \\ &= \frac{1}{2} m\, \mathbf{p}\cdot\mathbf{p} + m\, g\, \mathbf{e}_3\cdot\mathbf{q} = H(\mathbf{z})\ , \end{aligned} \tag{2.54}$$

which verifies, that H is invariant under rotations about the $\mathbf{e}_3$-axis. Consequently, the angular momentum with respect to the gravitational axis

$$L_3 = (\mathbf{q}\times\mathbf{p})\cdot\mathbf{e}_3\ , \tag{2.55}$$

is a conserved quantity during motions governed by the Hamiltonian equations of motion (2.27). Moreover, one can assume a translational action according to (2.44), such that the Hamiltonian becomes

$$H(\boldsymbol{\Phi}(\mathbf{g}(\alpha),\mathbf{z})) = \frac{1}{2} m\, \mathbf{p}\cdot\mathbf{p} + m\, g\, \mathbf{e}_3\cdot(\mathbf{q}+\alpha\boldsymbol{\xi}) = H(\mathbf{q},\mathbf{p}) + m\, g\, \mathbf{e}_3\cdot\alpha\boldsymbol{\xi}\ . \tag{2.56}$$

Both $\boldsymbol{\xi} = \mathbf{e}_1$ and $\boldsymbol{\xi} = \mathbf{e}_2$ lead to the G-invariance of the Hamiltonian. In view of (2.46), the linear momenta $J_1 = \mathbf{p}\cdot\mathbf{e}_1$ and $J_2 = \mathbf{p}\cdot\mathbf{e}_2$, respectively, are conserved quantities of the system. Hence, given a potential force into a certain direction reduces the conservation of linear momentum to the directions perpendicular to it.

2.3 Symplectic Hamiltonian Flow

Besides the conservation of momentum maps, the Hamiltonian structure gives rise to another conservation principle. When introducing flow maps in Section 2.3.1 we will also define the concept of *symplectic* maps. Next, we will show that the Hamiltonian flow map is symplectic and what consequences emanate from the symplectic geometry of the Hamiltonian phase space (cf. Sec. 2.3.2). Towards the end of this section, a short introduction to differential forms is given in Section 2.3.3 followed by a beneficial notation of symplecticness using the *wedge product*.

2.3.1 Flow Maps and Symplecticness

The following subsection is mostly taken from the textbook by Leimkuhler et al. [12].

The motion of a Hamiltonian system subject to the equations of motion (2.27) with appropriate initial condition $\mathbf{z}_0$ can be interpreted as a time-dependent mapping $\boldsymbol{\phi}_{t,H} : \mathcal{P} \to \mathcal{P}$ of the initial conditions onto the state at time t as

$$\mathbf{z}(t, \mathbf{z}_0) = \boldsymbol{\phi}_{t,H}(\mathbf{z}_0) \ . \tag{2.57}$$

Obviously, for $t = 0$ the initial state $\mathbf{z}_0$ is mapped onto itself. In general, this map is unknown but further analysis will provide some deeper understanding of Hamiltonian systems. The Jacobian $\mathbf{F}(t) \in \mathbb{R}^{2d \times 2d}$ is given by the gradient with respect to the phase space variable

$$\mathbf{F}(t) = \mathrm{D}_{\mathbf{z}} \boldsymbol{\phi}_{t,H}(\mathbf{z}_0) \ . \tag{2.58}$$

The application of the same gradient with respect to $\mathbf{z}$ in the equations of motion (2.27) yields

$$\mathrm{D}_{\mathbf{z}}(\dot{\mathbf{z}}(t)) = \mathrm{D}_{\mathbf{z}}(\mathbb{J}\mathrm{D}H(\boldsymbol{\phi}_{t,H}(\mathbf{z}_0)) = \mathbb{J}\mathrm{D}^2 H(\mathbf{z})\mathrm{D}_{\mathbf{z}}\boldsymbol{\phi}_{t,H}(\mathbf{z}_0) \tag{2.59}$$

with the Hessian (A.6) of H denoted as $\mathrm{D}^2 H(\mathbf{z}) \in \mathbb{R}^{2d \times 2d}$. Eventually, the interchange of spatial and temporal derivative on the left-hand side and considering the definition of the flow map Jacobian (2.58) on the right-hand side brings us to a matrix-valued differential equation for the Jacobian $\mathbf{F}(t)$, which reads

$$\dot{\mathbf{F}}(t) = \mathbb{J}\mathrm{D}^2 H(\mathbf{z}(t))\mathbf{F}(t) \tag{2.60}$$

with the initial condition $\mathbf{F}(t = 0) = \mathbf{I}_{2d \times 2d}$ being the unity matrix on $\mathbb{R}^{2d}$.

A map $\boldsymbol{\Psi} : \mathbb{R}^{2\mathrm{d}} \to \mathbb{R}^{2\mathrm{d}}$ is called *symplectic* if its Jacobian $\mathrm{D}\boldsymbol{\Psi}(\mathbf{z})$ satisfies

$$\mathrm{D}\boldsymbol{\Psi}(\mathbf{z})^{\mathrm{T}} \mathbb{J}^{-1} \mathrm{D}\boldsymbol{\Psi}(\mathbf{z}) = \mathbb{J}^{-1} \ , \tag{2.61}$$

for all $\mathbf{z}$ in the domain of definition of $\boldsymbol{\Psi}$ - given the invertible, constant and skew-symmetric structure matrix $\mathbb{J}$. For the special case of the canonical structure matrix from (2.28), the map is sometimes also termed as *canonical*. It can be easily proven that the Hamiltonian flow map (2.57) is symplectic. On the one hand, for $t = 0$ the condition above is satisfied since $\mathbf{I}\,\mathbb{J}^{-1}\,\mathbf{I} = \mathbb{J}^{-1}$. On the other hand, for $t > 0$ we can show that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{F}(t)\mathbb{J}^{-1}\mathbf{F}(t)\right) &= \mathbf{F}^{\mathrm{T}}\mathbb{J}^{-1}\dot{\mathbf{F}} + \dot{\mathbf{F}}^{\mathrm{T}}\mathbb{J}^{-1}\mathbf{F} \\ &= \mathbf{F}^{\mathrm{T}}\mathbb{J}^{-1}\left(\mathbb{J}\mathrm{D}^2 H(\mathbf{z}(t))\mathbf{F}\right) + \left(\mathbf{F}^{\mathrm{T}}\mathrm{D}^2 H(\mathbf{z}(t))\mathbb{J}^{\mathrm{T}}\right)\mathbb{J}^{-1}\mathbf{F} \\ &= \mathbf{F}^{\mathrm{T}}\left(\mathrm{D}^2 H(\mathbf{z}(t)) - \mathrm{D}^2 H(\mathbf{z}(t))\right)\mathbf{F} = \mathbf{0} \ , \end{aligned} \tag{2.62}$$

where (2.60) has been taken into account as well as the skew-symmetry of $\mathbb{J}$ and the

symmetry of the Hessian $\mathrm{D}^2 H(\mathbf{z})$. Thus, we can state that the Hamiltonian flow map is symplectic which can be expressed via

$$\mathbf{F}(t)^{\mathrm{T}} \mathbb{J}^{-1} \mathbf{F}(t) = \mathbb{J}^{-1} \ . \tag{2.63}$$

2.3.2 Symplectic Geometry of the Phase Space

For planar maps $\boldsymbol{\Psi}$ the Jacobian $\mathrm{D}\boldsymbol{\Psi}(\mathbf{z}) \in \mathbb{R}^{2\times 2}$ can be written as

$$\mathrm{D}\boldsymbol{\Psi}(\mathbf{z}) = \begin{bmatrix} \mathrm{D}\Psi_{11} & \mathrm{D}\Psi_{12} \\ \mathrm{D}\Psi_{21} & \mathrm{D}\Psi_{22} \end{bmatrix} \ . \tag{2.64}$$

By plugging this relation into the symplecticness-condition (2.61) we obtain

$$\mathrm{D}\Psi_{11}\,\mathrm{D}\Psi_{22} - \mathrm{D}\Psi_{12}\,\mathrm{D}\Psi_{21} = \det(\mathrm{D}\boldsymbol{\Psi}(\mathbf{z})) = 1 \ . \tag{2.65}$$

Consequently, symplectic planar maps have a determinat, which is everywhere equal to one. In analogy to the deformation gradient in elasticity theory for incompressible materials, the determinant of the Jacobian maps oriented areas $\mathcal{A}$ in the two-dimensional phase space as

$$\mathcal{A}(\mathcal{U}_t) = \int_{\mathcal{U}_t} \mathrm{d}q\,\mathrm{d}p = \int_{\mathcal{U}_0} \det(\mathrm{D}\boldsymbol{\Psi}(\mathbf{z}))\,\mathrm{d}q_0\,\mathrm{d}p_0 = \int_{\mathcal{U}_0} \mathrm{d}q_0\,\mathrm{d}p_0 = \mathcal{A}(\mathcal{U}_0) \ , \tag{2.66}$$

where $\mathcal{U}_t \subset \mathbb{R}^2$ denotes a bounded subset of the two dimensional phase space. Thus, a symplectic map of the plane is area preserving. A depiction can be found in Fig. 2.3. For $d > 1$ this property is equivalent to saying that the volume in phase space occupied by a neighborhood of points $\mathcal{U}_t \subset \mathbb{R}^{2d}$, transported by a map according to

$$\mathcal{U}_t = \boldsymbol{\Psi}(\mathcal{U}_0) = \left\{ \mathbf{z} \in \mathbb{R}^{2d} : \mathbf{z} = \boldsymbol{\Psi}(\mathbf{z}_0), \mathbf{z}_0 \in \mathcal{U}_0 \right\} \ , \tag{2.67}$$

is always equal to the initial volume occupied by $\mathcal{U}_0$. Remember that we have shown in (2.62), that the Hamiltonian flow map $\boldsymbol{\phi}_{t,H}$ is symplectic. Consequently, Hamiltonian dynamics preserve phase space volume during motion. Note that for higher dimensional cases, symplecticness implies also other invariants and cannot be reduced to volume preservation, only.

Entering the field of differential geometry, one can derive an alternative representation of the symplectic structure. Let us firstly introduce a bilinear and skew-symmetric function $\Omega : \mathbb{R}^{2d} \times \mathbb{R}^{2d} \to \mathbb{R}$ acting on two elements $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^{2d}$. Bilinearity refers to the fact that Ω is linear in both arguments. Skew-symmetry can be written as $\Omega(\boldsymbol{\xi}, \boldsymbol{\eta}) = -\Omega(\boldsymbol{\eta}, \boldsymbol{\xi})$, which is also referred to as a *two-form*. The canonical structure matrix introduced in (2.28) gives rise to the symplectic two-form

$$\Omega(\boldsymbol{\xi}, \boldsymbol{\eta}) = \boldsymbol{\xi} \cdot \mathbb{J}^{-1} \boldsymbol{\eta} \ . \tag{2.68}$$

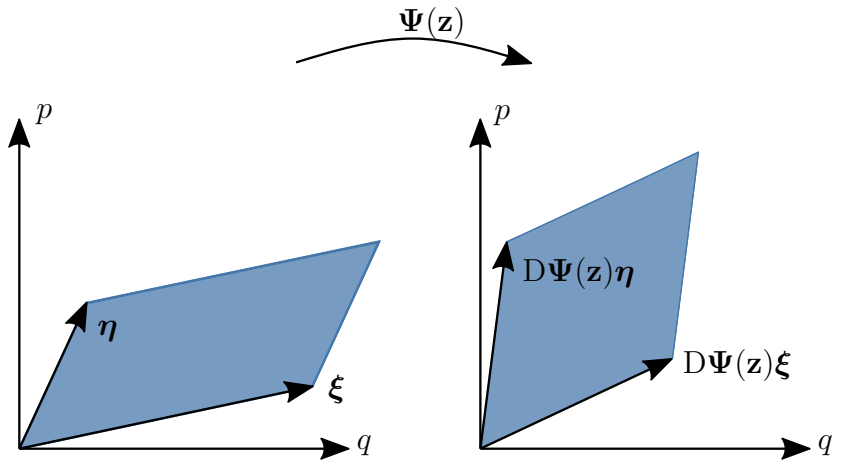

Figure 2.3: Symplectic area preservation for $d = 1$ (inspired by Hairer et al. [15])

In order to give a geometric interpretation, we can analyze once more the case $d = 1$ as depicted in Fig. 2.3: The two-form represents the oriented area spanned by the two vectors $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^2$. Denoting the planar two-form with a subscript "0" we have

$$\Omega_0(\boldsymbol{\xi}, \boldsymbol{\eta}) = \xi_2\eta_1 - \xi_1\eta_2 \ , \tag{2.69}$$

which can be interpreted as the oriented area spanned by $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$, computed with the cross-product of the two vectors. For $d > 1$, the two vectors can be projected into the (q_i, p_i)-coordinate plane, writing them as $\boldsymbol{\xi}^{(i)} \in \mathbb{R}^2$ and $\boldsymbol{\eta}^{(i)} \in \mathbb{R}^2$. Assuming an ordering as in the phase space vector (2.26), the components of $\boldsymbol{\xi}^{(i)}$ for example can be gained from the representation

$$\boldsymbol{\xi} = \begin{bmatrix} \xi_1^{(1)} & \xi_1^{(2)} & \dots & \xi_1^{(d)} & \xi_2^{(1)} & \xi_2^{(2)} & \dots & \xi_2^{(d)} \end{bmatrix}^{\mathrm{T}} \ . \tag{2.70}$$

Consequently, the symplectic two-form is given by the sum of the oriented areas for $i = 1, ..., d$ as

$$\Omega(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{i=1}^{d} \Omega_0(\boldsymbol{\xi}^{(i)}, \boldsymbol{\eta}^{(i)}) \ . \tag{2.71}$$

This is equivalent to the notation given in (2.68). This enables us to redefine symplectic maps in terms of the symplectic two-form: A map $\mathbf{\Psi} : \mathbb{R}^{2\mathrm{d}} \to \mathbb{R}^{2\mathrm{d}}$ is called *symplectic* if it leaves the symplectic two-form Ω invariant in the sense that

$$\Omega(\mathrm{D}\mathbf{\Psi}(\mathbf{z})\boldsymbol{\xi}, \mathrm{D}\mathbf{\Psi}(\mathbf{z})\boldsymbol{\eta}) = \Omega(\boldsymbol{\xi}, \boldsymbol{\eta}) \ , \tag{2.72}$$

where the original two-form is equal to the two-form of the transports of $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ under the linearization of $\mathbf{\Psi}$. Fig. 2.3 displays the mapping of elements $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ by $\mathbf{\Psi}$ and the preservation of the symplectic two-form, representing the oriented area for $d = 1$. Making use of the definition of the two-form in (2.68), the last equation can be written

as

$$\boldsymbol{\xi} \cdot \left(\mathrm{D}\boldsymbol{\Psi}(\mathbf{z})^{\mathrm{T}} \mathbb{J}^{-1} \mathrm{D}\boldsymbol{\Psi}(\mathbf{z}) - \mathbb{J}^{-1} \right) \boldsymbol{\eta} = 0 \ , \tag{2.73}$$

which verifies the initial definition of a symplectic map, which has been given in (2.61).

2.3.3 Differential Forms and Wedge Product

The following part dealing with differential forms mainly follows along the works by Arnold [4], Holm et al. [3] and Leimkuhler et al. [12].

Let $f : \mathcal{M} \to \mathbb{R}$ be a smooth scalar field on a differentiable manifold $\mathcal{M} \subset \mathbb{R}^n$. Then the *directional derivative* of f at $\mathbf{z} \in \mathcal{M}$ along $\boldsymbol{\xi} \in \mathcal{T}_{\mathbf{z}}\mathcal{M}$ is given by a linear map $\mathrm{d}f_{\mathbf{z}} : \mathcal{T}_{\mathbf{z}}\mathcal{M} \to \mathbb{R}$, defined by

$$\mathrm{d}f_{\mathbf{z}}(\boldsymbol{\xi}) := \frac{\mathrm{d}}{\mathrm{d}\varepsilon} f(\mathbf{z} + \varepsilon\boldsymbol{\xi})\Big|_{\varepsilon=0} = \mathrm{D}f(\mathbf{z}) \cdot \boldsymbol{\xi} \ . \tag{2.74}$$

Considering the individual components of the tangent vector $\boldsymbol{\xi}$ the directional derivative can be rewritten as

$$\mathrm{d}f_{\mathbf{z}}(\boldsymbol{\xi}) = \sum_{i=1}^{n} \frac{\partial f}{\partial z_i} \xi_i \tag{2.75}$$

(cf. Holm et al. [3] or Leimkuhler et al. [12]). The expression $\mathrm{d}f_{\mathbf{z}}(\bullet)$ is referred to as *differential* of f at $\mathbf{z}$ and represents a so-called differential *one-form*. If we assume the special case, in which the coordinate function $f(\mathbf{z}) = z_i$ is considered, then the directional derivative yields the important relation

$$\mathrm{d}z_i(\boldsymbol{\xi}) = \xi_i \ , \tag{2.76}$$

for $i = 1, ..., n$. Henceforth, the differentials $\mathrm{d}z_i$ can be used as a basis for the representation of the directional derivative of any smooth function f, viz.

$$\mathrm{d}f_{\mathbf{z}}(\boldsymbol{\xi}) = \sum_{i=1}^{n} \frac{\partial f}{\partial z_i} \, \mathrm{d}z_i(\boldsymbol{\xi}) \ . \tag{2.77}$$

Consequently, the *total differential* $\mathrm{d}f : \mathcal{T}\mathcal{M} \to \mathbb{R}$ is given by

$$\mathrm{d}f = \sum_{i=1}^{n} \frac{\partial f}{\partial z_i} \, \mathrm{d}z_i \tag{2.78}$$

and does not require any arguments. On the contrary, the directional derivative (2.77) depends on a certain choice of $\boldsymbol{\xi}$ (cf. Arnold [4]).

The present topic becomes clear with an example taken from Arnold [4] with $\mathcal{M} = \mathbb{R}$ and $f(z) = z^2$ as depicted in Fig. 2.4. On the one hand, the total differential $\mathrm{d}f = 2z \, \mathrm{d}z$ depends on the point z and on the tangent vector $\xi = \mathrm{d}z$. On the other hand the

directional derivative $\mathrm{d}f_{\mathbf{z}}(\xi)$ requires a specific evaluation. If $z = 1$ and $\xi = 2$ for example, we obtain $\mathrm{d}f_{\mathbf{z}}(\xi) = 4$.

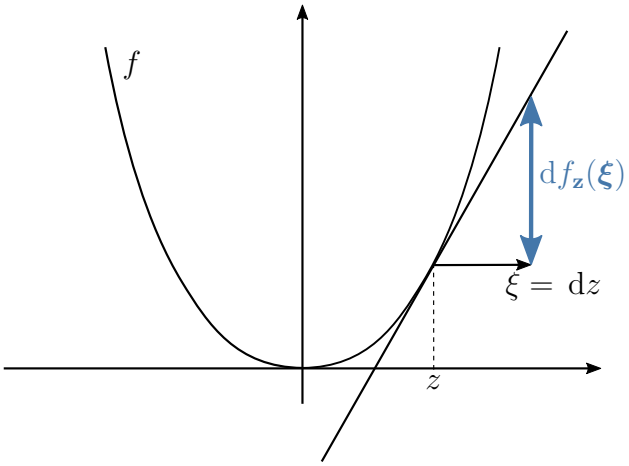

Figure 2.4: Differential and directional derivative of $f : \mathbb{R} \to \mathbb{R}, z \mapsto z^2$

Considering the brief vector notation for differential one-forms $\mathrm{d}\mathbf{z} = [\,\mathrm{d}z_1, \mathrm{d}z_2, ..., \mathrm{d}z_n]^{\mathrm{T}}$, it is possible to rewrite the total differential (2.78) as

$$\mathrm{d}f = \mathrm{D}f(\mathbf{z}) \cdot \mathrm{d}\mathbf{z} \; . \tag{2.79}$$

Furthermore, if $\mathbf{z}$ belongs to the phase space $\mathcal{P} \subset \mathbb{R}^{2d}$, the total differential $\mathrm{d}f : \mathcal{P} \to \mathbb{R}$ is given by

$$\mathrm{d}f = \sum_{i=1}^{d} \frac{\partial f}{\partial q_i} \mathrm{d}q_i + \sum_{i=1}^{d} \frac{\partial f}{\partial p_i} \mathrm{d}p_i \; , \tag{2.80}$$

where $\mathrm{d}\mathbf{q}$ and $\mathrm{d}\mathbf{p}$ accumulate the differential one-forms acting on $\boldsymbol{\xi} \in \mathcal{P}$ defined by

$$\mathrm{d}q_i(\boldsymbol{\xi}) = \xi_1^{(i)} \; , \tag{2.81a}$$

$$\mathrm{d}p_i(\boldsymbol{\xi}) = \xi_2^{(i)} \; . \tag{2.81b}$$

Note that the respective components $\xi_1^{(i)}$ and $\xi_2^{(i)}$ are for example given by the structure (2.70) and (2.26). Furthermore, the differential (2.80) can be rewritten in vector notation as

$$\mathrm{d}f = \mathrm{D}_1 f(\mathbf{q}, \mathbf{p}) \cdot \mathrm{d}\mathbf{q} + \mathrm{D}_2 f(\mathbf{q}, \mathbf{p}) \cdot \mathrm{d}\mathbf{p} \; . \tag{2.82}$$

Moreover, the wedge product of two differential one-forms $\mathrm{d}\mathbf{a} \in \mathbb{R}^d$ and $\mathrm{d}\mathbf{b} \in \mathbb{R}^d$ acting on any two vectors $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{R}^{2d}$ can be defined by

$$(\,\mathrm{d}\mathbf{a} \wedge \mathrm{d}\mathbf{b})(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{i=1}^{d} (\,\mathrm{d}a_i \wedge \mathrm{d}b_i)\,(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{i=1}^{d} (\,\mathrm{d}b_i(\boldsymbol{\xi})\,\mathrm{d}a_i(\boldsymbol{\eta}) - \mathrm{d}a_i(\boldsymbol{\xi})\,\mathrm{d}b_i(\boldsymbol{\eta})) \tag{2.83}$$

(cf. Leimkuhler et al. [12]). Note that crucial properties of the wedge product are given in Appendix A.2. Thus, the symplectic two form (2.71) can be rewritten in terms of the

wedge product as

$$\Omega(\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{i=1}^{d} \mathrm{d}q_i \wedge \mathrm{d}p_i \, (\boldsymbol{\xi}, \boldsymbol{\eta}) \ , \tag{2.84}$$

where the differential one-forms $\mathrm{d}q_i$, $\mathrm{d}p_i$ of the phase space coordinates defined in (2.81) have been taken into account. Omitting the arguments, the symplectic two-form can be rewritten more briefly in vector notation as

$$\Omega = \mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} \ . \tag{2.85}$$

Note that this representation is only a briefer notation of (2.84) that still accounts for the summation of the wedge product of scalar one-forms. Eventually, the symplecticness of a map on the phase space $(\hat{\mathbf{q}}, \hat{\mathbf{p}}) = \boldsymbol{\Psi}(\mathbf{q}, \mathbf{p})$ can be expressed as

$$\mathrm{d}\hat{\mathbf{q}} \wedge \mathrm{d}\hat{\mathbf{p}} = \mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} \ . \tag{2.86}$$

Remembering that Hamiltonian flow maps are symplectic, it is equivalent to say that the symplectic two-form (2.85) is conserved along solutions of the Hamiltonian equations of motions (2.27):

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega = 0 \ , \tag{2.87}$$

which can be derived by temporal differentiation of the definition of the wedge product (2.83) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega = \frac{\mathrm{d}}{\mathrm{d}t} \left(\mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} \right) = \mathrm{d}\dot{\mathbf{q}} \wedge \mathrm{d}\mathbf{p} + \mathrm{d}\mathbf{q} \wedge \mathrm{d}\dot{\mathbf{p}} \ . \tag{2.88}$$

The conservation of Ω by Hamiltonian systems is easily verified for the the canonical Hamiltonian equations of motions (2.14). The differential one-forms corresponding to $\dot{\mathbf{q}}$ and $\dot{\mathbf{p}}$ can be deduced as

$$\mathrm{d}\dot{\mathbf{q}} = \mathrm{D}^2_{21} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{q} + \mathrm{D}^2_{22} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{p} \ , \tag{2.89a}$$

$$\mathrm{d}\dot{\mathbf{p}} = -\mathrm{D}^2_{11} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{q} - \mathrm{D}^2_{12} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{p} \ , \tag{2.89b}$$

where $\mathrm{D}^2_{ij}(\bullet)$ denotes the second-order partial derivative (A.5). Eventually, the temporal evolution of Ω becomes

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Omega = {} & \mathrm{D}^2_{22} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{p} \wedge \mathrm{d}\mathbf{p} - \mathrm{d}\mathbf{q} \wedge \mathrm{D}^2_{11} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{q} \\ & + \mathrm{D}^2_{21} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} - \mathrm{d}\mathbf{q} \wedge \mathrm{D}^2_{12} H(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{p} = 0 \ . \end{aligned} \tag{2.90}$$

Note that $\mathrm{D}^2_{11} H$ and $\mathrm{D}^2_{22} H$ both are symmetric matrices (cf. relation (A.6)), such that the first and second term in the last equation vanish due to property of the wedge product for matrix multiplication with symmetric matrices (A.16). Moreover, the last two terms cancel each other out because of the symmetry of the Hessian of H. Additionaly, the

matrix-multiplication property of the wedge product (A.15) yields

$$\mathrm{D}^2_{21}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q}\wedge\,\mathrm{d}\mathbf{p} = \left(\mathrm{D}^2_{12}H(\mathbf{q},\mathbf{p})\right)^{\mathrm{T}}\mathrm{d}\mathbf{q}\wedge\,\mathrm{d}\mathbf{p} = -\,\mathrm{d}\mathbf{q}\wedge\mathrm{D}^2_{12}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p}\ . \tag{2.91}$$

2.4 Variational Integrators

After having shown the variational principles and conservation properties of dynamical systems in the previous section we now proceed by giving an overview of the concept of variational integrators in order to solve dynamical systems numerically. The following fundamentals on variational integrators can be found for example in Lew et al. [18] or Hairer et al. [15]. In Section 2.4.1 we will cover the general idea of variational integrators. In Section 2.4.2 discrete conditions for the conservation of the symplectic strucuture and the momentum maps are given. Towards the end of this part in Section 2.4.3, the symplectic Euler method will be explained as an example.

2.4.1 General Idea and Governing Equations

We start by considering a dynamical problem over a time period of $\mathcal{I} = [0\,,\,T]$. This interval can be subdivided into N subintervals of the constant time step size $h \in \mathbb{R}^+$, viz.

$$\mathcal{I} = \bigcup_{n=0}^{N-1} [t^n\ ,\ t^{n+1}] \tag{2.92}$$

with $t^0 = 0$ and $t^N = T$ such that $h = t^{n+1} - t^n$. Most classical integration schemes are based on the direct discretization of the equations of motion (2.31) as

$$\mathbf{z}^{n+1} - \mathbf{z}^n = h\,\mathbf{X}^{\mathrm{d}}_{\mathrm{H}}(\mathbf{z}^n, \mathbf{z}^{n+1})\ , \tag{2.93}$$

by introducing some discrete Hamiltonian vector field $\mathbf{X}^{\mathrm{d}}_{\mathrm{H}}$. Accounting for the initial conditions of the dynamical system, one has to state $\mathbf{z}_0 = \mathbf{z}(t = 0)$. However, this procedure can lead to some undesirable issues, i.e. conservation laws or symmetries of the time-continuous problems are not inherited by the approximate solutions of the time-stepping scheme.

Another way to derive time integration schemes, which can alleviate those issues, is the concept of *variational integrators*, whose main idea is to take one step back and approximate the underlying variational principle instead. For a Lagrangian framework, the action integral (2.3) can be discretized as

$$S(\mathbf{q}) = \int_0^T L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\,\mathrm{d}t = \sum_{n=0}^{N-1}\int_{t^n}^{t^{n+1}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\,\mathrm{d}t \approx \sum_{n=0}^{N-1} L_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = S_{\mathrm{d}}(\{\mathbf{q}^n\}_0^N)\ , \tag{2.94}$$

where L_d is an approximation of the integral of L on the subinterval $[t^n\,,\,t^{n+1}]$ as

$$L_\mathrm{d}(\mathbf{q}^n,\mathbf{q}^{n+1}) \approx \int_{t^n}^{t^{n+1}} L(\mathbf{q}(t),\dot{\mathbf{q}}(t))\,\mathrm{d}t \tag{2.95}$$

and $\mathbf{q}^n \approx \mathbf{q}(t^n)$ can be viewed as an approximation of the time-continuous solution evaluated at t^n. There exist multiple numerical methods to approximate the integral of a function over a given interval, by making use of the function evaluated at certain points, e.g. midpoint-rule, trapezoidal rule and many more. Given a specific choice of L_d a discrete version of Hamilton's principle of least action extremizes the discrete action integral, viz.

$$\delta S_\mathrm{d}(\{\mathbf{q}^n\}_0^N) = \sum_{n=0}^{N-1} \delta L_\mathrm{d}(\mathbf{q}^n,\mathbf{q}^{n+1}) = 0\ , \tag{2.96}$$

where the first variation of L_d can be computed by the chain rule such that

$$\sum_{n=0}^{N-1} \Big(\mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^n,\mathbf{q}^{n+1})\cdot\delta\mathbf{q}^n + \mathrm{D}_2 L_\mathrm{d}(\mathbf{q}^n,\mathbf{q}^{n+1})\cdot\delta\mathbf{q}^{n+1}\Big) = 0\ . \tag{2.97}$$

Note that the endpoint conditions (2.6) for variations of $\mathbf{q}$ directly apply to the discrete versions such that

$$\delta\mathbf{q}^0 = \delta\mathbf{q}^N = \mathbf{0}\ . \tag{2.98}$$

Thus, by splitting up the sum in (2.97), employing an index shift for the second term and considering the last property (2.98), one obtains

$$\sum_{n=1}^{N-1} \Big(\mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^n,\mathbf{q}^{n+1}) + \mathrm{D}_2 L_\mathrm{d}(\mathbf{q}^{n-1},\mathbf{q}^n)\Big)\cdot\delta\mathbf{q}^n = 0\ . \tag{2.99}$$

As the discrete variations just like the continuous ones are assumed to be arbitrary, this eventually yields the *discrete Euler-Lagrange equations* (DEL)

$$\mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^n,\mathbf{q}^{n+1}) + \mathrm{D}_2 L_\mathrm{d}(\mathbf{q}^{n-1},\mathbf{q}^n) = \mathbf{0}\ , \tag{2.100}$$

for $n = 1, ..., N-1$, which are discrete counterparts of the Lagrangian Equations of the Second Kind (2.7) and serve as a time-stepping scheme. In general, this set of equations is implicit and thus requires a numerical solution method such as Newton's method. It is moreover possible, that the DEL can be brought into the form (2.93) as well.

Note that the previous considerations have been conducted in a Lagrangian framework, assuming that the velocities are discretized by means of discrete $\mathbf{q}^n$ as well. Typically, one makes use of discrete differences, e.g. $\dot{\mathbf{q}}(t^n) \approx (\mathbf{q}^{n+1}-\mathbf{q}^n)/h$. In order to achieve a Hamiltonian description one either has to define discrete momenta apriori (cf. Hairer et

al. [15]) such that

$$\mathbf{p}^n := -\mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}) \ , \tag{2.101a}$$
$$\mathbf{p}^{n+1} := \mathrm{D}_2 L_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}) \ , \tag{2.101b}$$

which are the discrete counterparts of (2.10) and are therefore referred to as *discrete fiber derivative*. Or a different ansatz is chosen, which discretizes the mixed Livens principle (2.18), such that the discrete fiber derivative directly emerges from the DEL of the variational integrator and do not have to be defined a priori.

2.4.2 Discrete Conservation Principles

In any case, it is possible to achieve a Hamiltonian or mixed framework $(\mathbf{q}^n, \mathbf{p}^n) \mapsto (\mathbf{q}^{n+1}, \mathbf{p}^{n+1})$ which allows for one-step integration methods with a discrete flow map $\Psi_h : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ defined by

$$\mathbf{z}^{n+1} = \Psi_h(\mathbf{z}^n) \ , \tag{2.102}$$

which is in general nonlinear and may only be defined implicitly by the solution of the correspoding DEL (cf. Leimkuhler et al. [12]). Recall that a map is said to be symplectic if (2.61) holds. For the present case this yields

$$\left(\mathrm{D}\Psi_h(\mathbf{z}^n)\right)^\mathrm{T} \mathbb{J}^{-1} \left(\mathrm{D}\Psi_h(\mathbf{z}^n)\right) = \mathbb{J}^{-1} \ . \tag{2.103}$$

Examples on how to check the symplecticness with that condition can be found for example in Hairer et al. [15]. However, Ψ_h may not always be given explicitly. Thus, it can be beneficial to consider another representation making use of the wedge product. A numerical integration scheme is called symplectic, if the discrete condition

$$\mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n = \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} \ . \tag{2.104}$$

is satisfied by the integrators DEL. This condition can be viewed as the discrete version of (2.87). The well-known explicit Euler method is an example for integration schemes based on the direct approximation of the equations of motion by assuming a discrete Hamiltonian vector field, as in (2.93). As can be seen in Fig. 2.5, this method is not symplectic and therefore does not preserve the area in phase space. The symplectic Euler method on the contrary represents a symplectic, variational integrator and preserves the area in phase space. We refer to the upcoming Sec. 2.4.3 for further details. Fig. 2.5, which has been taken from Hairer et al. [15], displays the phase space diagrams for a mathematical pendulum described in minimal coordinates.

Integration schemes of the form (2.93) inherit the conservation of at most quadratic momentum maps $J_{\boldsymbol{\xi}}$ defined in (2.40) if

$$J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1}) - J_{\boldsymbol{\xi}}(\mathbf{z}^n) = \mathrm{D}J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1/2}) \cdot (\mathbf{z}^{n+1} - \mathbf{z}^n) = h\mathrm{D}J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1/2}) \cdot \mathbf{X}_\mathrm{H}^\mathrm{d}(\mathbf{z}^n, \mathbf{z}^{n+1}) = 0 \ , \tag{2.105}$$

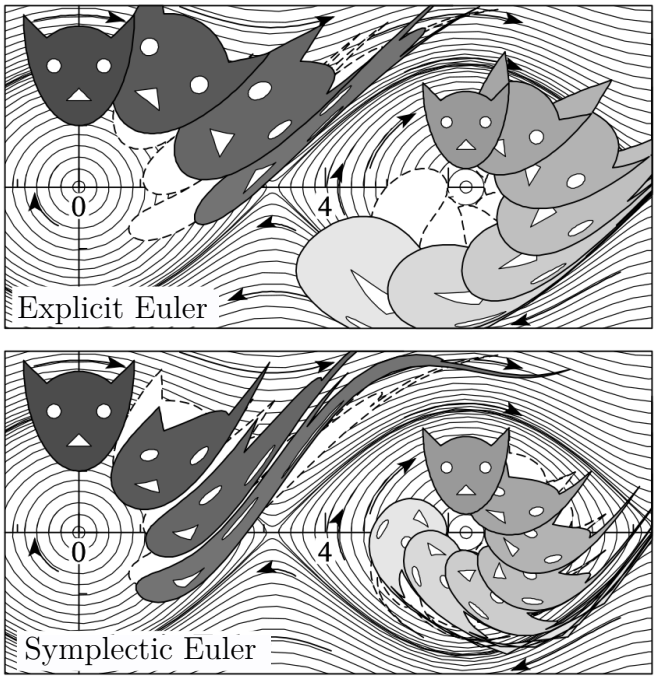

Figure 2.5: Area preservation of symplectic and non-symplectic time-stepping schemes, taken from Hairer et al. [15]

is true in every time step. Note that we have assumed the form (2.93) for the DEL. Moreover, this leads to the discrete conservation of the Hamiltonian if

$$H(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}) - H(\mathbf{q}^n, \mathbf{p}^n) = 0 \ . \tag{2.106}$$

2.4.3 Symplectic Euler Method

As already mentioned above, the symplectic Euler method (see e.g. Leimkuhler et al. [12]) can be obtained as a variational integrator based on Livens principle (2.18). There are two different ways leading to a so-called Euler A method and Euler B method, respectively. The symplectic Euler B method emanates for example from a discrete action integral given by

$$\tilde{S}_\mathrm{d} = \sum_{n=0}^{N-1} \left[h\, L(\mathbf{q}^n, \mathbf{v}^n) + \mathbf{p}^{n+1} \cdot \left(\mathbf{q}^{n+1} - \mathbf{q}^n - h\, \mathbf{v}^n \right) \right] + \mathbf{p}^0 \cdot (\mathbf{q}^0 - \bar{\mathbf{q}}) \ , \tag{2.107}$$

where the additional Lagrangian multiplier $\mathbf{p}^0$ enforces the initial configuration. Discrete stationarity conditions are applied to the discrete action integral, leading to

$$\sum_{n=0}^{N-1} \delta\mathbf{p}^{n+1} \cdot \left(\mathbf{q}^{n+1} - \mathbf{q}^n - h\, \mathbf{v}^n \right) = 0 \ , \tag{2.108a}$$

$$\sum_{n=0}^{N-1} \delta\mathbf{v}^n \cdot \left(h\, \mathrm{D}_2 L(\mathbf{q}^n, \mathbf{v}^n) - h\, \mathbf{p}^{n+1} \right) = 0 \ , \tag{2.108b}$$

along with

$$\sum_{n=0}^{N-1} \Big(\delta\mathbf{q}^n \cdot h\, \mathrm{D}_1 L(\mathbf{q}^n, \mathbf{v}^n) + \mathbf{p}^{n+1} \cdot (\delta\mathbf{q}^{n+1} - \delta\mathbf{q}^n) \Big) + \delta\mathbf{q}^0 \cdot \mathbf{p}^0 = 0 \ . \tag{2.108c}$$

Applying an index shift and considering the endpoint conditions (2.98) for the discrete variations $\delta\mathbf{q}^n$ yields the DEL of the symplectic Euler B method as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{v}^n \ , \tag{2.109a}$$
$$\mathbf{p}^{n+1} - \mathbf{p}^n = h\, \mathrm{D}_1 L(\mathbf{q}^n, \mathbf{v}^n) \ , \tag{2.109b}$$
$$\mathbf{p}^{n+1} = \mathrm{D}_2 L(\mathbf{q}^n, \mathbf{v}^n) \ , \tag{2.109c}$$

for $N = 0, ..., N-1$. Note that the conjugate momenta emerge directly from the discrete action integral and do not have to be defined a priori as mentioned in (2.101). If we assume a typical Lagrangian with constant mass matrix (2.8) and eliminate velocities by making use of the discrete fiber derivative (2.109c), we obtain

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{M}^{-1} \mathbf{p}^{n+1} \ , \tag{2.110a}$$
$$\mathbf{p}^{n+1} - \mathbf{p}^n = -h\, \mathrm{D}V(\mathbf{q}^n) \ , \tag{2.110b}$$

for $N = 0, ..., N-1$. We can now prove, that this method is indeed symplectic by means of (2.104). Making use of the skew-symmetry of the wedge product (A.13) one can deduce that

$$\mathrm{d}\mathbf{p}^{n+1} \wedge (\, \mathrm{d}\mathbf{q}^{n+1} - \mathrm{d}\mathbf{q}^n) + (\, \mathrm{d}\mathbf{p}^{n+1} - \mathrm{d}\mathbf{p}^n) \wedge \mathrm{d}\mathbf{q}^n = \mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n - \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} \ . \tag{2.111}$$

Plugging in the DEL of the Euler B method (2.110) yields

$$\mathrm{d}\mathbf{p}^{n+1} \wedge \mathbf{M}^{-1}\, \mathrm{d}\mathbf{p}^{n+1} - \mathrm{D}^2 V(\mathbf{q}^n)\, \mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{q}^n = \mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n - \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} \ . \tag{2.112}$$

Making use of the property of the wedge product for symmetric matrix multiplication (A.16) gives rise to the fact that both terms on the left-hand side of the last equation vanish, since $\mathbf{M}^{-1}$ and $\mathrm{D}^2 V(\mathbf{q}^n)$ are symmetric matrices. Thus, the discrete condition for symplectic methods is satisfied, viz.

$$\mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n = \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} \ . \tag{2.113}$$

3 Constrained Dynamical Systems

In the previous chapter the analysis of dynamical systems has been covered, including variational principles, equations of motion, symmetries and momentum maps as well as symplectic structure and the numerical, temporal integration. In some cases however, those systems might be subject to certain constraints. We will see that the presence of constraints will not alter the main ideas on the whole but some modifications have to be considered. After introducing holonomic constraints, adapting the variational principles to them and analyzing the previously derived conservation principles in the presence of constraints in Section 3.1, the topic of *differential-algebraic equations* will be covered in Section 3.2. Consequently, the concept of variational integrators can be applied to systems with constraints as well, which will be demonstrated in Section 3.3. In the last section of this chapter (cf. Sec. 3.4) a framework for the analysis of rigid bodies will be provided, such that the generic DAEs for constrained dynamics from Sec. 3.1 can be applied.

3.1 Fundamental Dynamics with Holonomic Constraints

Firstly, the description of constraints both on configuration level (*primary constraints*) and on velocity level (*secondary constraints*) will be covered in Section 3.1.1. Furthermore, the variational principles derived previously will be modified to account for constraints in Section 3.1.2 and pertinent conservation laws will be discussed in Section 3.1.3. The crucial fundamentals can be found for example in Marsden et al. [19].

3.1.1 Holonomic Constraints and Constraint Manifolds

Let us consider a d-dimensional dynamical system with redundant coordinates $\mathbf{q} \in \mathcal{Q}$ with $\mathcal{Q} \subset \mathbb{R}^d$, that are subject to m independent holonomic constraints $g_k : \mathcal{Q} \times \mathbb{R} \to \mathbb{R}$, which can be comprised in a column vector, such that

$$\mathbf{g}(\mathbf{q}, t) = \mathbf{0} \ . \tag{3.1}$$

In particular, throughout this thesis we consider only constraint functions, which do not depend on time explicitly. Thus, one speaks of *scleronomic* holonomic constraints $\mathbf{g} : \mathcal{Q} \to \mathbb{R}^m$ defined by

$$\mathbf{g}(\mathbf{q}) = \mathbf{0} \ . \tag{3.2}$$

The dependence on time only occurs implicitly since $\mathbf{q} = \mathbf{q}(t)$. Otherwise the constraint function is referred to as *rheonomic* holonomic. Since all constraint functions shall be independent, the gradient (A.2) of the constraint vector, for which we define the abbreviation

$$\mathbf{G}(\mathbf{q}) = \mathrm{D}\mathbf{g}(\mathbf{q}) \ , \tag{3.3}$$

is of rank m. As (3.2) is true for any point in time, the time derivative has to vanish accordingly. Thus the so-called *consistency condition* reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{g}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0} \ . \tag{3.4}$$

The last relation is referred to as constraint *on velocity level* or *secondary constraint*. Later, it will become clear that this statement can be interpreted as an orthogonality condition between constraint forces and velocity vector. On the contrary, (3.2) is referred to as constraint on *configuration level* or *primary constraint*. The motion of the dynamical system, which underlies the constraints, is now restricted to the so-called *constraint manifold*

$$\mathcal{C} = \{\mathbf{q}(t) \in \mathcal{Q} : \mathbf{g}(\mathbf{q}) = \mathbf{0}\} \subset \mathcal{Q} \ , \tag{3.5}$$

which is a $(d-m)$-dimensional submanifold of the configuration manifold $\mathcal{Q}$ of the system without constraints (cf. Leyendecker [47]), defined in Section 2.1.1. Likewise, corresponding velocity vectors $\dot{\mathbf{q}}$ belong to the constraint tangent space

$$\mathcal{T}_{\mathbf{q}}\mathcal{C} = \{\dot{\mathbf{q}} \in \mathcal{T}_{\mathbf{q}}\mathcal{Q} : \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = 0\} \subset \mathcal{T}_{\mathbf{q}}\mathcal{Q} \ . \tag{3.6}$$

Accordingly, the set $(\mathbf{q}, \dot{\mathbf{q}})$ is henceforth restricted to the $2(d-m)$-dimensional constraint tangent bundle

$$\mathcal{TC} = \{(\mathbf{q}, \dot{\mathbf{q}}) \in \mathcal{TQ} : \mathbf{g}(\mathbf{q}) = \mathbf{0}, \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0}\} \subset \mathcal{TQ} \ , \tag{3.7}$$

where the tangent bundle $\mathcal{TQ}$ has been introduced in Section 2.1.1 as well.

3.1.2 Variational Principle and Governing Equations

In order to force the system into the constrained solution, Lagrange multipliers $\lambda_k \in \mathbb{R}$ with $k = 1, ..., m$ are introduced to enforce the primary constraint (3.2). These Lagrange multipliers can be accumulated in a vector $\boldsymbol{\lambda} \in \mathrm{R}^m$ and are integrated into Hamilton's principle (2.5) by introducing an augmented Lagrangian $L^{\boldsymbol{\lambda}} : \mathcal{TQ} \times \mathbb{R}^m \to \mathbb{R}$ that reads

$$L^{\boldsymbol{\lambda}}(\mathbf{q}, \dot{\mathbf{q}}) = L(\mathbf{q}, \dot{\mathbf{q}}) - \boldsymbol{\lambda} \cdot \mathbf{g}(\mathbf{q}) \ . \tag{3.8}$$

Hamilton's principle of least action for constrained systems thus reads

$$\delta S^{\boldsymbol{\lambda}} = \int_0^T \delta L^{\boldsymbol{\lambda}}(\mathbf{q}, \dot{\mathbf{q}})\, \mathrm{d}t = 0 \ . \tag{3.9}$$

Note that similar to the unconstrained case the variational principle assumes arbitrary variations $\delta\mathbf{q}$ satisfying the endpoint conditions, viz.

$$\delta\mathbf{q}(t=0) = \delta\mathbf{q}(t=T) = \mathbf{0} \ . \tag{3.10}$$

Solving (3.9) involves moreover also the variation with respect to $\boldsymbol{\lambda}$ and eventually leads to the constrained EL equations

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathrm{D}_2 L(\mathbf{q}, \dot{\mathbf{q}}) - \mathrm{D}_1 L(\mathbf{q}, \dot{\mathbf{q}}) + \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{0} \ , \tag{3.11a}$$

$$\mathbf{g}(\mathbf{q}) = \mathbf{0} \ , \tag{3.11b}$$

which are usually termed *Lagrange's equations of the first kind*. The set of equations represents *differential-algebraic equations*, shortly referred to as *DAEs*. In (3.11a) the term $\mathbf{G}^{\mathrm{T}}\boldsymbol{\lambda}$ represents additional forces acting on the system, called *constraint forces*. The k-th coordinate $\mathrm{D}g_{\mathrm{k}}$ determines the direction of the constraint force whereas the corresponding Lagrange multiplier λ_{k} adapts its magnitude, such that (3.11a) and (3.11b) are satisfied by $(\mathbf{q}, \dot{\mathbf{q}}) \in \mathcal{TC}$.

As for unconstrained systems, the kinematic constraint $\dot{\mathbf{q}} = \mathbf{v}$ can be enforced by using the Lagrange multiplier method in the sense of a Livens principle (cf. (2.18)) for constrained systems. An augmented action integral, emanating from that idea, is given by

$$\tilde{S}^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{v}, \mathbf{p}, \boldsymbol{\lambda}) = \int_0^T \left(L(\mathbf{q}, \mathbf{v}) - \boldsymbol{\lambda} \cdot \mathbf{g}(\mathbf{q}) + \mathbf{p} \cdot (\dot{\mathbf{q}} - \mathbf{v})\right) \mathrm{d}t \ , \tag{3.12}$$

which can be seen as a direct modification of (2.18) for constrained systems. The equations of motion can be directly derived by demanding the stationarity $\delta\tilde{S}^{\boldsymbol{\lambda}} = 0$, accounting for endpoint conditions (3.10), and considering the arbitrariness of the variations $\delta\mathbf{q}$,$\delta\mathbf{v}$, $\delta\mathbf{p}$ and $\delta\boldsymbol{\lambda}$. Thus, the extremum of (3.12) is given by the solutions of the DAEs

$$\dot{\mathbf{q}} = \mathbf{v} \ , \tag{3.13a}$$

$$\dot{\mathbf{p}} = \mathrm{D}_1 L(\mathbf{q}, \mathbf{v}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \ , \tag{3.13b}$$

$$\mathbf{p} = \mathrm{D}_2 L(\mathbf{q}, \mathbf{v}) \ , \tag{3.13c}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{q}) \ . \tag{3.13d}$$

As for unconstrained systems a corresponding Hamiltonian formalism can be gained by

introducing an augmented Hamiltonian $H^{\boldsymbol{\lambda}} : \mathcal{P} \times \mathbb{R}^m \to \mathbb{R}$ as

$$H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p}) + \boldsymbol{\lambda} \cdot \mathbf{g}(\mathbf{q}) \ , \tag{3.14}$$

which can be derived with the help of a Legendre transformation of the augmented Lagrangian (3.8) in an analogous way as for unconstrained systems (cf. Sec. 2.1.2). As $(\mathbf{q}, \dot{\mathbf{q}}) \in \mathcal{TC}$, within the Hamiltonian formalism $(\mathbf{q}, \mathbf{p})$ belong to the *constrained phase space* $\mathcal{P}_\mathrm{c}$ such that the secondary constraint becomes a function of the momentum

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{g}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} = \mathbf{0} \ . \tag{3.15}$$

Thus, $(\mathbf{q}, \mathbf{p})$ must fulfill both constraints (3.18c) and (3.15) which define the constraint phase space $\mathcal{P}_\mathrm{c}$ as

$$\mathcal{P}_\mathrm{c} = \left\{(\mathbf{q}, \mathbf{p}) \in \mathcal{P} : \mathbf{g}(\mathbf{q}) = \mathbf{0}, \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} = \mathbf{0}\right\} \subset \mathcal{P} \ , \tag{3.16}$$

which is identical with the *constraint cotangent bundle*, viz. $\mathcal{P}_\mathrm{c} = \mathcal{T}^*\mathcal{C}$. Consequently, the Hamiltonian equations of motion taking account of holonomic constraints read

$$\dot{\mathbf{q}} = +\mathrm{D}_2 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \ , \tag{3.17a}$$
$$\dot{\mathbf{p}} = -\mathrm{D}_1 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \ , \tag{3.17b}$$
$$\mathbf{0} = +\mathrm{D}_{\boldsymbol{\lambda}} H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \ . \tag{3.17c}$$

If we evaluate the derivatives for a typical dynamical system with the standard Hamiltonian given in (2.15), the DAEs become

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p} \ , \tag{3.18a}$$
$$\dot{\mathbf{p}} = -\mathrm{D}V(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \ , \tag{3.18b}$$
$$\mathbf{0} = \mathbf{g}(\mathbf{q}) \ . \tag{3.18c}$$

Note that the Lagrangian formulation (3.11), the mixed formulation in the sense of Livens principle (3.13) and the Hamiltonian formulation (3.18) are all equivalent concerning the solution curves $\mathbf{q}(t)$.

3.1.3 Symmetries and Conservation Laws

In Section 2.1.2 it has been shown that the Hamiltonian H is a first integral of unconstrained dynamical systems (cf. Eq. (2.17)). This property is directly inherited by constrained systems subject to the equations of motion in (3.17) and can be easily shown in an analogous manner by temporal derivative of the augmented Hamiltonian

$$\begin{aligned}
\dot{H}^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) &= \mathrm{D}_1 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \cdot \dot{\mathbf{q}} + \mathrm{D}_2 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \cdot \dot{\mathbf{p}} + \mathrm{D}_{\boldsymbol{\lambda}} H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \cdot \dot{\boldsymbol{\lambda}} \\
&= \mathrm{D}_1 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \cdot \mathrm{D}_2 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) - \mathrm{D}_2 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) \cdot \mathrm{D}_1 H^{\boldsymbol{\lambda}}(\mathbf{q}, \mathbf{p}) + \mathbf{0} \cdot \dot{\boldsymbol{\lambda}} \\
&= 0 \ ,
\end{aligned} \tag{3.19}$$

where (3.17a) and (3.17b) have been taken into account to replace $\dot{\mathbf{q}}$ and $\dot{\mathbf{p}}$, respectively. Considering that the constraint (3.18c) is identically zero at every time, we can deduce that the standard Hamiltonian (2.15) itself is conserved along solutions of the constrained Hamiltonian equations, viz. $\dot{H}(\mathbf{q},\mathbf{p}) = 0$. Moreover, it can be demonstrated that also the symplectic structure of Hamiltonian systems can be carried over to constrained systems. The following deductions are taken from Leimkuhler et al. [12]. We start by writing the total differential (2.79) of the constraint on configuration level (3.2) as

$$\mathrm{d}\mathbf{g}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\,\mathrm{d}\mathbf{q} = \mathbf{0}\ . \tag{3.20}$$

The differential one-forms, emanating as the total differentials of the equations of motion (3.17a) to (3.17c), are given by

$$\mathrm{d}\dot{\mathbf{q}} = \mathrm{D}^2_{21}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} + \mathrm{D}^2_{22}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p}\ , \tag{3.21a}$$

$$\mathrm{d}\dot{\mathbf{p}} = -\mathrm{D}^2_{11}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} - \mathrm{D}^2_{12}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p} - \mathrm{d}\left(\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right)\ , \tag{3.21b}$$

$$\mathbf{0} = \mathbf{G}(\mathbf{q})\,\mathrm{d}\mathbf{q}\ , \tag{3.21c}$$

where we used the chain rule for functions depending on $\mathbf{q}$ and $\mathbf{p}$ given in (2.80). Next, we compute the temporal derivative of the canonical symplectic two-form (2.88) as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Omega =&\ \mathrm{d}\dot{\mathbf{q}} \wedge \mathrm{d}\mathbf{p} + \mathrm{d}\mathbf{q} \wedge \mathrm{d}\dot{\mathbf{p}} \\ =&\ \mathrm{D}^2_{22}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p} \wedge \mathrm{d}\mathbf{p} - \mathrm{d}\mathbf{q} \wedge \mathrm{D}^2_{11}H(\mathbf{q},\mathbf{p}\,\mathrm{d}\mathbf{q}) - \mathrm{d}\left(\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right) \wedge \mathrm{d}\mathbf{q} \\ &+ \mathrm{D}^2_{21}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} - \mathrm{d}\mathbf{q} \wedge \mathrm{D}^2_{12}H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p}\ ,\end{aligned} \tag{3.22}$$

where we have substituted (3.21a) and (3.21b). Analogously to the unconstrained equations of motion, we can argue in the sense of (2.91) and employ properties of the wedge product to cancel out the terms depending on the Hamiltonian. The remaining part can be written as

$$\begin{aligned}\mathrm{d}\left(\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right) \wedge \mathrm{d}\mathbf{q} &= \mathbf{G}(\mathbf{q})^{\mathrm{T}}\,\mathrm{d}\boldsymbol{\lambda} \wedge \mathrm{d}\mathbf{q} + \sum_{\mathrm{k}=1}^{\mathrm{m}} \lambda_{\mathrm{k}}\mathrm{D}^2 g_{\mathrm{k}}(\mathbf{q})\,\mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{q} \\ &= \mathrm{d}\boldsymbol{\lambda} \wedge \mathbf{G}(\mathbf{q})\,\mathrm{d}\mathbf{q} \\ &= 0\ ,\end{aligned} \tag{3.23}$$

where in the first subequation we were able to cancel the second term as the Hessian of the k-th constraint is a symmetric matrix (cf. relation (A.16)). For the first term we applied the matrix multiplication property of the wedge product (A.15) such that the differential of the primary constraint (3.20) can be taken into account. Eventually, we have shown that the symplectic two-form Ω is conserved along solutions of the DAEs of constrained dynamical systems.

3.2 Differential-Algebraic Equations of Constrained Dynamics

As we have seen in Section 3.1.2 the equations of motion, which govern constrained dynamics in redundant coordinates, represent DAEs. The *differentiation index* will be introduced in Section 3.2.1 and explained by means of the constrained Hamiltonian equations of motion in Section 3.2.2. This section also presents ways of reducing the differentiation index which can lead to beneficial results. Lastly, the commonly used *GGL stabilization* will be shown in Section 3.2.3.

3.2.1 Differentiation Index

Constrained equations of motion formulated in redundant coordinates represent DAEs, which can be generically written as

$$\mathbf{h}(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0} \ , \tag{3.24}$$

where $\mathbf{x}$ is a vector accumulating all independent variables. For this kind of DAEs the *differentiation index* $\nu \in \mathbb{N}_0$ when existing is defined as follows: The minimal number of differentiations of $\mathbf{h}$ that one has to perform in order to arrive at an ordinary differential equation which can be brought into a certain explicit form $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$, where $\mathbf{f}$ denotes the right-hand side of the explicit ODE (cf. Yoshimura [49]). This formalism can be written as

$$\mathbf{h}(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0} \rightsquigarrow \dot{\mathbf{h}}(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0} \rightsquigarrow ... \rightsquigarrow \frac{\mathrm{d}^{(\nu)}}{\mathrm{d}t^{(\nu)}} \mathbf{h}(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0} \Leftrightarrow \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \ . \tag{3.25}$$

The explicit ODE $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ is referred to as *underlying ODE* and has the same solutions as the original problem (cf. Kunkel et al. [13]). The differentiation index is invariant under global transformations. Thus, it remains the same for the Lagrangian formulation with $\mathbf{x} = [\mathbf{q},\ \dot{\mathbf{q}},\ \boldsymbol{\lambda}]$, for the Hamiltonian formulation with $\hat{\mathbf{x}} = [\mathbf{q},\ \mathbf{p},\ \boldsymbol{\lambda}]^{\mathrm{T}}$ and for the Livens formulation, in which the generic state variable is $\tilde{\mathbf{x}} = [\mathbf{q},\ \mathbf{v},\ \mathbf{p},\ \boldsymbol{\lambda}]^{\mathrm{T}}$.

3.2.2 Index Reduction of Constrained Hamiltonian DAEs

By the definition of the differentiation index the configuration-level DAEs derived in the previous section have index $\nu = 3$. This can be demonstrated exemplarily for the Hamiltonian formulation whose configuration-level DAEs are given by (3.18). The secondary constraint emanates from temporal differentiation of the constraint as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{g}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} = \mathbf{0} \ , \tag{3.26}$$

which represents the first of three differentiations. By replacing the primary constraint equation with this constraint on momentum-level, the momentum-level DAEs read

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p} \ , \tag{3.27a}$$
$$\dot{\mathbf{p}} = -\mathrm{D}V(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \ , \tag{3.27b}$$
$$\mathbf{0} = \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} \ , \tag{3.27c}$$

which then only have index $\nu = 2$. For a second time we proceed by temporal differentiation. The constraint on acceleration level thus reads

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathbf{g}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\dot{\mathbf{p}} + \dot{\mathbf{G}}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} = \mathbf{0} \ , \tag{3.28}$$

where the time derivative of the constraint gradient (in index notation) can be computed as

$$\dot{G}_{\mathrm{ij}} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial g_i}{\partial q_j}\right) = \frac{\partial^2 g_i}{\partial q_j \partial q_k}\dot{q}_k \ . \tag{3.29}$$

Eventually, it is possible to plug in (3.27a) and (3.27b) for $\dot{\mathbf{q}}$ and $\dot{\mathbf{p}}$, respectively, such that we arrive at the constraint on acceleration level

$$\mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\left(-\mathrm{D}V(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right) + \mathrm{D}^2\mathbf{g}(\mathbf{q}) : \left((\mathbf{M}^{-1}\mathbf{p}) \otimes (\mathbf{M}^{-1}\mathbf{p})\right) = \mathbf{0} \ . \tag{3.30}$$

From the last equation some algebraic conversions yield an explicit form for the Lagrange multipliers $\boldsymbol{\lambda} = \boldsymbol{\Lambda}(\mathbf{q}, \mathbf{p})$ given as

$$\boldsymbol{\Lambda}(\mathbf{q}, \mathbf{p}) = \left(\mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{G}(\mathbf{q})^{\mathrm{T}}\right)^{-1}\left[\mathrm{D}^2\mathbf{g}(\mathbf{q}) : \left((\mathbf{M}^{-1}\mathbf{p}) \otimes (\mathbf{M}^{-1}\mathbf{p})\right) - \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathrm{D}V(\mathbf{q})\right] \ . \tag{3.31}$$

By considering this last equation in our DAEs we have an acceleration-level formulation

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p} \ , \tag{3.32a}$$
$$\dot{\mathbf{p}} = -\mathrm{D}V(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \ , \tag{3.32b}$$
$$\boldsymbol{\lambda} = \boldsymbol{\Lambda}(\mathbf{q}, \mathbf{p}) \ , \tag{3.32c}$$

which then only have differentiation index $\nu = 1$. This can easily be verified since it is possible to take the time-derivative of the explicit formulation for the Lagrange multiplier (3.31) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Lambda}(\mathbf{q}, \mathbf{p}) = \mathrm{D}_1\boldsymbol{\Lambda}(\mathbf{q}, \mathbf{p})\dot{\mathbf{q}} + \mathrm{D}_2\boldsymbol{\Lambda}(\mathbf{q}, \mathbf{p})\dot{\mathbf{p}} \ , \tag{3.33}$$

which is the third and last temporal differentiation. Again, $\dot{\mathbf{q}}$ and $\dot{\mathbf{p}}$ can be replaced such that the underlying ODE is given by

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p} \ , \tag{3.34a}$$

$$\dot{\mathbf{p}} = -\mathrm{D}V(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \ , \tag{3.34b}$$

$$\dot{\boldsymbol{\lambda}} = \mathrm{D}_1\boldsymbol{\Lambda}(\mathbf{q},\mathbf{p})\mathbf{M}^{-1}\mathbf{p} - \mathrm{D}_2\boldsymbol{\Lambda}(\mathbf{q},\mathbf{p})\left(\mathrm{D}V(\mathbf{q}) + \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right) \ , \tag{3.34c}$$

or briefly $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ as required in the definition of the differentiation index (3.25).

Research has shown that the index 3 formulation (3.18) on configuration level is prone to numerical instability (cf. Yoshimura [49]). In particular, the system may become numerically ill-conditioned when singular points exist. This issue can be alleviated by considering the index 2 formulation on momentum level (3.27) or the index 1 formulation on acceleration level (3.32). Those formulations however induce violations of the primary constraint on configuration level $\mathbf{g}(\mathbf{q}) = \mathbf{0}$, which are referred to as *drift phenomena*. They occur in a larger magnitude for the acceleration-level formulation than for the momentum-level formulation.

3.2.3 GGL Stabilization

Gear, Gupta and Leimkuhler introduced a method to account for the numerical ill-conditions without having the drawback of drift. By means of an *index reduction by minimal extension* new variables are considered such that the system of equations of motion is extended and the differentiation index drops to $\nu = 2$ (cf. Gear et al. [50]). This method was later on baptized *GGL stabilization*.

The main idea of the stabilization method is to couple the secondary constraint into the dynamics by making use of additional Lagrange multipliers $\boldsymbol{\gamma} \in \mathbb{R}^m$. Thus, for a Hamiltonian formulation the kinematic equation is modified as

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p} + \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma} \tag{3.35}$$

in analogy to the structure of the equation for $\dot{\mathbf{p}}$. The final DAEs based on a Hamiltonian viewpoint with reduced index $\nu = 2$ are given by

$$\dot{\mathbf{q}} = \mathbf{M}^{-1}\mathbf{p} + \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma} \ , \tag{3.36a}$$

$$\dot{\mathbf{p}} = -\mathrm{D}V(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \ , \tag{3.36b}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{q}) \ , \tag{3.36c}$$

$$\mathbf{0} = \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} \ . \tag{3.36d}$$

Ever since, this method has been commonly used and is thus of big importance. Numerical methods can be constructed directly by discretizing the DAEs (3.36). Due to the modification of the kinematic equation, the system loses its Hamiltonian structure. Thus, it requires a bit more effort to show the symmetries of the GGL system. Let

us first verify, whether the Hamiltonian H is still a conserved quantity. We start by differentiating the standard Hamiltonian (2.15) with respect to time

$$\begin{aligned}\dot{H} &= \mathrm{D}_1 H(\mathbf{q},\mathbf{p}) \cdot \dot{\mathbf{q}} + \mathrm{D}_2 H(\mathbf{q},\mathbf{p}) \cdot \dot{\mathbf{p}} \\ &= \mathrm{D}V(\mathbf{q}) \cdot \left(\mathbf{M}^{-1}\mathbf{p} + \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}\right) + \mathbf{M}^{-1}\mathbf{p} \cdot \left(-DV(\mathbf{q}) - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right) \ , \end{aligned} \tag{3.37}$$

where (3.36a) and (3.36b) are taken into account. The terms without Lagrange multipliers cancel each other out and the term with $\boldsymbol{\lambda}$ vanishes due to the secondary constraint (3.36d). Thus, we obtain

$$\dot{H} = \mathrm{D}V(\mathbf{q}) \cdot \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma} \ . \tag{3.38}$$

It appears that the conservation of H is not given a priori. However, one can show that the consistency condition requires the newly introduced Lagrange multiplier $\boldsymbol{\gamma}$ to become zero. We can show this with

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{g}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0} \ , \tag{3.39}$$

where we can substitute $\dot{\mathbf{q}}$ by (3.36a) such that

$$\mathbf{G}(\mathbf{q})\left(\mathbf{M}^{-1}\mathbf{p} + \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}\right) = \mathbf{0} \ . \tag{3.40}$$

The first addend vanishes due to (3.36d). Eventually, we arrive at the condition

$$\mathbf{G}(\mathbf{q})\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma} = \mathbf{0} \ , \tag{3.41}$$

where $\mathbf{G}(\mathbf{q})\mathbf{G}(\mathbf{q})^{\mathrm{T}}$ is non-singular for k independent constraint functions. Thus, $\boldsymbol{\gamma} = \mathbf{0}$ is true for all t. Eventually, we can verify that the Hamiltonian is a conserved quantity along solutions of the GGL method (3.36). Moreover, the symplecticness of the GGL DAEs has to be analyzed. A straightforward proof starts by computing the temporal derivative of the symplectic two-form as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Omega &= \mathrm{d}\dot{\mathbf{q}} \wedge \mathrm{d}\mathbf{p} + \mathrm{d}\mathbf{q} \wedge \mathrm{d}\dot{\mathbf{p}} \\ &= \left(\mathbf{M}^{-1}\,\mathrm{d}\mathbf{p} + \mathrm{d}(\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma})\right) \wedge \mathrm{d}\mathbf{p} - \mathrm{d}\mathbf{q} \wedge \left(\mathrm{D}^2 V(\mathbf{q})\,\mathrm{d}\mathbf{q} + \mathrm{d}(\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda})\right) \ . \end{aligned} \tag{3.42}$$

Once more (3.36a) and (3.36b) are used to replace $\dot{\mathbf{q}}$ and $\dot{\mathbf{p}}$, respectively. Due to the symmetric matrix multiplication property (A.16) the first and third term vanish. As we have demonstrated in (3.23) also the second term becomes zero. Eventually, we arrive at

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Omega &= \mathrm{d}(\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}) \wedge \mathrm{d}\mathbf{p} \\ &= \mathbf{G}(\mathbf{q})^{\mathrm{T}}\,\mathrm{d}\boldsymbol{\gamma} \wedge \mathrm{d}\mathbf{p} + \sum_{\mathrm{k}=1}^{\mathrm{m}} \gamma_{\mathrm{k}} \mathrm{D}^2 g_{\mathrm{k}}(\mathbf{q})\,\mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} \ . \end{aligned} \tag{3.43}$$

Therefore, the conservation of symplectic two-form Ω along solutions of the equations of

motion of the GGL method (3.36a) to (3.36d) depends on the Lagrange multiplier $\boldsymbol{\gamma}$ as well. As we have shown in (3.41) that $\boldsymbol{\gamma}$ vanishes, the GGL DAEs are symplectic.

Note that the relation $\boldsymbol{\gamma} = \mathbf{0}$ simply leads to the fact that the GGL method reduces to the standard DAEs (3.18a) to (3.18c) on configuration level. However, the DAEs derived in the framework of the GGL stabilisation allow for a variety of new time integration methods. But note that the loss of the Hamiltonian structure of the DAEs can lead to the fact that GGL stabilized integration schemes might not be symplectic in a discrete sense, since $\boldsymbol{\gamma}^n = \mathbf{0}$ is in general not identically verified.

3.3 Integration Methods for Constrained Systems

This short section will firstly demonstrate how variational integrators are constructed in the case of constrained dynamics in Section 3.3.1. Furthermore, we show an example integrator derived accordingly (cf. Sec. 3.3.2). And in the last part of this section, we apply the GGL stabilization from Section 3.2.3 to this variational integration scheme in Section 3.3.3.

3.3.1 Variational Integrators for Constrained Systems

For constrained dynamical systems the procedure of generating a variational integrator is done according to Section 2.4. However, it is crucial to consider the augmented Lagrangian (3.8) instead, such that a discrete action integral can be exemplarily given by

$$S_{\mathrm{d}}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{q}^{n+1}, \boldsymbol{\lambda}^{n+1}) = \sum_{n=0}^{N-1} \left(L_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) - \boldsymbol{\lambda}^{n+1} \cdot \mathbf{g}_{\mathrm{d}}(\mathbf{q}^{n+1}) \right) , \tag{3.44}$$

where $\mathbf{g}_{\mathrm{d}}$ denotes an approximation of the primary constraints. The discrete stationarity conditions yield constrained DEL as

$$\mathrm{D}_1 L_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) + \mathrm{D}_2 L_{\mathrm{d}}(\mathbf{q}^{n-1}, \mathbf{q}^n) - \mathrm{D}\mathbf{g}_{\mathrm{d}}^{\mathrm{T}}(\mathbf{q}^n)\boldsymbol{\lambda}^n = \mathbf{0} , \tag{3.45a}$$

$$\mathbf{g}_{\mathrm{d}}(\mathbf{q}^{n+1}) = \mathbf{0} , \tag{3.45b}$$

for $n = 1, ..., N-1$ where $\mathrm{D}\mathbf{g}_{\mathrm{d}}^{\mathrm{T}}$ is a discrete version of the constraint gradient $\mathbf{G}(\mathbf{q})$. Hamiltonian formulations or other choices of unknowns can be considered in an analogous manner by taking care of the additional unknowns in the discrete variational principle.

3.3.2 Constrained Symplectic Euler

A variational integrator for constrained dynamics can be achieved by considering the Livens principle for constrained dynamics given in (3.12). A straightforward discretiza-

tion of the action integral reads

$$\tilde{S}_{\mathrm{d}}^{\boldsymbol{\lambda}} = \sum_{n=0}^{N-1} \Big[h\, L(\mathbf{q}^n, \mathbf{v}^n) - h\, \boldsymbol{\lambda}^{n+1} \cdot \mathbf{g}(\mathbf{q}^{n+1}) + \mathbf{p}^{n+1} \cdot \Big(\mathbf{q}^{n+1} - \mathbf{q}^n - h\, \mathbf{v}^n \Big) \Big] + \mathbf{p}^0 \cdot (\mathbf{q}^0 - \bar{\mathbf{q}}) - h\, \boldsymbol{\lambda}^0 \cdot \mathbf{g}(\mathbf{q}^0) \ , \tag{3.46}$$

where we make use of additional Lagrange multipliers $\mathbf{p}^0$ and $\boldsymbol{\lambda}^0$ in order to enforce the initial configuration and that this configuration satisfies the primary constraint, respectively. The following procedure involves the stationarity conditions $\delta \tilde{S}_{\mathrm{d}}^{\boldsymbol{\lambda}} = 0$, taking account of the discrete endpoint conditions (2.98) and considering the arbitrariness of all variations and has already been shown in Sec. (2.4.3) for the unconstrained case. For the present integrator one has to demand stationarity with respect to the Lagrange multiplier $\boldsymbol{\lambda}$ as well. Eventually. we can write the DEL as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{v}^n \ , \tag{3.47a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = h\, \mathrm{D}_1 L(\mathbf{q}^n, \mathbf{v}^n) - h\, \mathbf{G}(\mathbf{q}^n)^{\mathrm{T}} \boldsymbol{\lambda}^n \ , \tag{3.47b}$$

$$\mathbf{p}^{n+1} = \mathrm{D}_2 L(\mathbf{q}^n, \mathbf{v}^n) \ , \tag{3.47c}$$

$$\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{0} \ , \tag{3.47d}$$

for $n = 0, ..., N-1$. These relations represent discrete counterparts of the continuous DAEs previously derived in (3.13a) to (3.13d). Assuming a typical mechanical system with constant mass matrix, the Lagrangian is given in (2.8) and the discrete equations of motion (3.47a) to (3.47d) yield the time stepping scheme

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{M}^{-1} \mathbf{p}^{n+1} \ , \tag{3.48a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = -h\, \mathrm{D}V(\mathbf{q}^n) - h\, \mathbf{G}(\mathbf{q}^n)^{\mathrm{T}} \boldsymbol{\lambda}^n \ , \tag{3.48b}$$

$$\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{0} \ , \tag{3.48c}$$

for $n = 0, ..., N-1$, where we have eliminated the velocities. The above equations (3.48) represent a set of $2d + m$ relations for the unknowns $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}, \boldsymbol{\lambda}^n)$, which can be solved with Newton's method in every time step. Note that the structure of this integration scheme differs from the symplectic Euler B method (2.110) only with respect to the constraint equation and corresponding constraint forces in (3.48b). It can thus be regarded as a generalization of the symplectic Euler B method for constrained systems.

3.3.3 Classical Time Integration based on the GGL Stabilization

Based on the integration scheme introduced in the last Section 3.3.2, one can now employ the GGL stabilization (cf. Section 3.2.3) with ease. Accordingly, the discrete kinematic equation provided of the previous scheme (3.48a) has to be modified in the sense of (3.35). Eventually, the discrete kinematic equation of the GGL-stabilized scheme is given by

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{M}^{-1} \mathbf{p}^{n+1} + h\, \mathbf{G}(\mathbf{q}^n)^{\mathrm{T}} \boldsymbol{\gamma}^n \ , \tag{3.49}$$

where the Lagrange multipliers $\boldsymbol{\gamma}^{n+1}$ represent additional unknowns in every time step. Thus, in the sense of the GGL stabilization the secondary constraint in momentum formulation is coupled into the discrete equations of motion. Hence, one integration scheme based on the GGL stabilization is subject to

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\,\mathbf{M}^{-1}\mathbf{p}^{n+1} + h\,\mathbf{G}(\mathbf{q}^n)^{\mathrm{T}}\boldsymbol{\gamma}^n \;, \tag{3.50a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = -h\,\mathrm{D}V(\mathbf{q}^n) - h\,\mathbf{G}(\mathbf{q}^n)^{\mathrm{T}}\boldsymbol{\lambda}^n \;, \tag{3.50b}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{q}^{n+1}) \;, \tag{3.50c}$$

$$\mathbf{0} = \mathbf{G}(\mathbf{q}^{n+1})\mathbf{M}^{-1}\mathbf{p}^{n+1} \;, \tag{3.50d}$$

and serve as the discrete counterparts of the GGL equations of motion presented in (3.36a) to (3.36d). With respect to (3.48) the set of equations has been extended to $2(d+m)$ relations for the unknowns $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}, \boldsymbol{\lambda}^n, \boldsymbol{\gamma}^n)$ in every time step.

3.4 Rigid Bodies in Director Formulation

This work employs the rigid body formulation used by Betsch et al. (cf. [54] and [55]), Leyendecker [47], Krenk [57] and many others. This formulation enables us to apply the framework of DAEs for constrained dynamics which has been shown in the previous sections and circumvents the usage of angular velocities and accelerations in the equations of motion. However, it can be shown that the underlying description is equivalent to the well-known Newton-Euler equations for rigid bodies (cf. Leyendecker [47] or Betsch et al. [54]).

Consider a rigid body with *reference configuration* $\mathcal{B}_0 \subset \mathbb{R}^3$ at time $t = 0$ as depicted in Fig. 3.1. During motion, material points $\mathbf{X} \in \mathcal{B}_0$ are mapped to their spatial placement $\mathbf{x} \in \mathcal{B}$, where $\mathcal{B}$ denotes the *current configuration* at time $t > 0$. Besides the globally fixed, orthonormal basis $\{\mathbf{e}_i\}$, the present formulation employs a right-handed body frame $\{\mathbf{d}_i\}$ located in the *center of mass* of the body. The so-called *directors* $\mathbf{d}_i, i = 1, 2, 3$ are fixed to the body and therefore move with it during motion. For $t = 0$, we assume that the director frame's direction coincides with the global basis. Thus, we obtain

$$\{\mathbf{d}_i\}(t = 0) = \{\mathbf{e}_i\} \;. \tag{3.51}$$

Moreover, let the director body frame be aligned with the body's principle axes. It is crucial that the material coordinates X_i are defined relative to the origin of the director frame. Hence, the definition of the *center of mass* is given by

$$\int_{\mathcal{B}} X_i\,\rho(\mathbf{X})\,\mathrm{dV} = 0 \tag{3.52}$$

with $\rho : \mathcal{B}_0 \to \mathbb{R}^+$ being the material mass density. It is expedient to introduce a vector to the center of mass of the rigid body $\boldsymbol{\varphi} : \mathbb{R} \to \mathbb{R}^3$. Due to the rigidity of the body, every

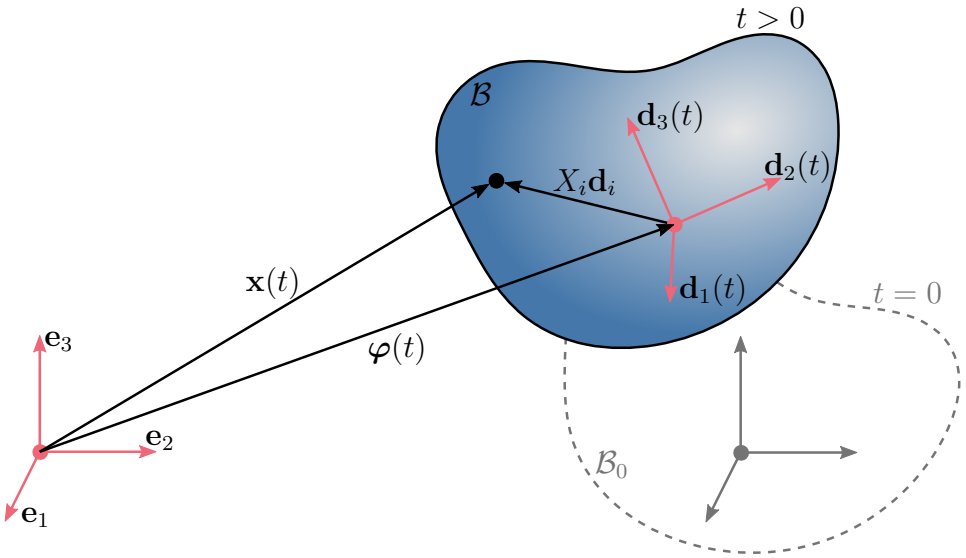

Figure 3.1: Spatial motion of a rigid body with director formulation

point on $\mathcal{B}$ is uniquely defined by its material coordinates X_i with respect to the director frame's origin such that we are able to express the spatial placement as a function of the material coordinates and time, viz.

$$\mathbf{x}(\mathbf{X}, t) = \boldsymbol{\varphi}(t) + X_i \mathbf{d}_i(t) \ . \tag{3.53}$$

The time dependence of the directors can be expressed by means of a rotational matrix $\mathbf{R} : \mathbb{R} \to SO(3)$ with $\mathbf{R}(0) = \mathbf{I}_{3\times 3}$ as

$$\mathbf{d}_i(t) = \mathbf{R}(t)\mathbf{e}_i \quad \text{or} \quad (d_i)_j = R_{jk}(e_i)_k \tag{3.54}$$

Taking into account that the k-th component of $\mathbf{e}_i$ is equal to the Kronecker symbol δ_{ik} we obtain $(d_i)_j = R_{ji}$. Thus, we find a representation of $\mathbf{R}$ with respect to the global $\{\mathbf{e}_i\}$ basis as

$$\mathbf{R}(t) = \begin{bmatrix} \mathbf{d}_1(t) & \mathbf{d}_2(t) & \mathbf{d}_3(t) \end{bmatrix} \ . \tag{3.55}$$

The relation (3.54) in its index notation can be multiplied by the l-th component of $\mathbf{e}_i$ which yields another representation of the rotational matrix (3.55) as

$$\mathbf{R}(t) = \sum_{i=1}^{3} \mathbf{d}_i(t) \otimes \mathbf{e}_i \ . \tag{3.56}$$

In view of (3.54), we can proceed by recasting the relation for the spatial coordinates introduced in (3.53) such that

$$\mathbf{x}(\mathbf{X}, t) = \boldsymbol{\varphi}(t) + \mathbf{R}(t)\mathbf{X} \ , \tag{3.57}$$

where the material point $\mathbf{X} = X_i \mathbf{e}_i$ does not depend on time. The kinetic energy at time t is defined as

$$T(t) = \frac{1}{2} \int_{\mathcal{B}_0} \dot{\mathbf{x}}(\mathbf{X}, t) \cdot \dot{\mathbf{x}}(\mathbf{X}, t) \rho(\mathbf{X}) \, \mathrm{dV} \ . \tag{3.58}$$

The spatial velocities are easily given by temporal derivative (A.1) of (3.53). This yields

$$\dot{\mathbf{x}}(\mathbf{X}, t) = \dot{\boldsymbol{\varphi}}(t) + \dot{\mathbf{R}}(t)\mathbf{X} \ . \tag{3.59}$$

Plugging that into the definition of the kinetic energy (3.58), it is possible to split T into a translatory and a rotational contribution since all coupled terms vanish in view of (3.52). Thus,

$$T(t) = T_{\mathrm{trans}}(t) + T_{\mathrm{rot}}(t) \ , \tag{3.60}$$

where the translatory part is given by

$$T_{\mathrm{trans}}(t) = \frac{1}{2} m \dot{\boldsymbol{\varphi}}(t) \cdot \dot{\boldsymbol{\varphi}}(t) \tag{3.61}$$

with the total mass

$$m = \int_{\mathcal{B}_0} \rho(\mathbf{X}) \, \mathrm{dV} \ . \tag{3.62}$$

The rotational part becomes

$$T_{\mathrm{rot}}(t) = \frac{1}{2} \int_{\mathcal{B}_0} (\dot{\mathbf{R}}(t)\mathbf{X}) \cdot (\dot{\mathbf{R}}(t)\mathbf{X}) \rho(\mathbf{X}) \, \mathrm{dV} \ . \tag{3.63}$$

Since $\dot{\mathbf{R}}$ does not depend on the reference configuration, it is admissible to pull it out of the integral. Moreover, it is expedient to introduce the convected Euler tensor

$$\mathbf{E} = \int_{\mathcal{B}_0} \mathbf{X} \otimes \mathbf{X} \rho(\mathbf{X}) \, \mathrm{dV} \tag{3.64}$$

such that the rotational kinetic energy becomes

$$T_{\mathrm{rot}}(t) = \frac{1}{2} \mathbf{E} : \dot{\mathbf{R}}(t)^{\mathrm{T}} \dot{\mathbf{R}}(t) \ . \tag{3.65}$$

For the sake of simplicity we can assume that the basis $\{\mathbf{e}_i\}$ coincides with the principle axes of $\mathcal{B}_0$. Thus, the convected Euler tensor is given by its spectral decomposition with its principal values E_i on the diagonal

$$\mathbf{E} = \sum_{i=1}^{3} E_i \mathbf{e}_i \otimes \mathbf{e}_i \quad \text{with} \quad E_i = \int_{\mathcal{B}_0} X_i^2 \, \rho(\mathbf{X}) \, \mathrm{dV} \ . \tag{3.66}$$

As the Euler tensor can be linked to the convected inertia tensor $\mathbf{J}$ according to

$$\mathbf{J} = (\operatorname{tr} \mathbf{E})\mathbf{I} - \mathbf{E} \ , \tag{3.67}$$

the principle values of the Euler tensor can be computed with the principal moments of inertia as $E_i = 1/2\,(J_j + J_k - J_i)$ for even permutations of the indices (i, j, k). The spectral decomposition (3.66) and the temporal differentiation of (3.56) give rise to an even simpler representation of the rotational kinetic energy in terms of the directors as

$$T_{\mathrm{rot}}(t) = \frac{1}{2} \sum_{i=1}^{3} E_i \, \dot{\mathbf{d}}_i(t) \cdot \dot{\mathbf{d}}_i(t) \ . \tag{3.68}$$

Eventually, it is possible to describe the motion of a rigid body by $n = 3 + 9 = 12$ redundant coordinates accumulated in the coordinate vector

$$\mathbf{q} = \begin{bmatrix} \boldsymbol{\varphi} \\ \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \end{bmatrix} \ . \tag{3.69}$$

This framework consequently allows for a representation of the system's Lagrangian in the standard fashion (2.8) with the constant and diagonal mass matrix

$$\mathbf{M} = \begin{bmatrix} m\mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & E_1\mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & E_2\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & E_3\mathbf{I} \end{bmatrix} \ . \tag{3.70}$$

The constraint configuration manifold is therefore defined by

$$\mathcal{C} = \left\{ \mathbf{q} \in \mathbb{R}^{12} : \mathbf{g}(\mathbf{q}) = \mathbf{0} \right\} \ , \tag{3.71}$$

which is subject to $m = 6$ holonomic constraints on configuration level. The primary constraints enforce the directors to stay orthonormal for all times due to the rigidity of the body

$$\mathbf{g}(\mathbf{q}) = \tilde{\mathbf{g}}(\{\mathbf{d}_{\mathrm{i}}\}) = \begin{bmatrix} \frac{1}{2}(\mathbf{d}_1 \cdot \mathbf{d}_1 - 1) \\ \frac{1}{2}(\mathbf{d}_2 \cdot \mathbf{d}_2 - 1) \\ \frac{1}{2}(\mathbf{d}_3 \cdot \mathbf{d}_3 - 1) \\ \mathbf{d}_1 \cdot \mathbf{d}_2 \\ \mathbf{d}_1 \cdot \mathbf{d}_3 \\ \mathbf{d}_2 \cdot \mathbf{d}_3 \end{bmatrix} = \mathbf{0} \ . \tag{3.72}$$

Note that this constraint can be alternatively expressed in terms of the rotational matrix $\mathbf{R}$. As it is directly linked to the directors by (3.55), the rigidity constraints can also be written as

$$\mathbf{g}(\mathbf{q}) = \hat{\mathbf{g}}(\mathbf{R}) = \frac{1}{2} \left(\mathbf{R}^{\mathrm{T}}\mathbf{R} - \mathbf{I}_{3\times 3} \right) = \mathbf{0} \ . \tag{3.73}$$

The last representation of the constraint gives rise to an interpretation of the rotational matrix as a deformation gradient tensor

$$\mathbf{R}(t) = \mathrm{D}_1\mathbf{x}(\mathbf{X}, t) \ , \tag{3.74}$$

which can be verified considering the motion mapping (3.57). It is to mention that the constrained formulation for rigid bodies, which has been demonstrated in this section, can be viewed as a special case of the *Cosserat theory* for deformable solids, when applying the rigidity constraint (3.73). For further details see Betsch [56].

4 A Novel Framework for Constrained Dynamical Systems

After covering the fundamentals of dynamical systems without constraints (cf. Chapter 2) and with constraints (cf. Chapter 3), the current part will introduce a novel variational framework to describe constrained dynamical systems considering both primary and secondary constraints. The structure of this new variational principle will be covered in Section 4.1.

Furthermore, based on the newly proposed functional we want to construct three different time integration methods based on the following approaches:

I Straigtforwardly discretize the novel functional generalizing the symplectic Euler B method (cf. Sec. 4.2).

II Derive a variational integrator based on a more complex discretization of the novel functional employing auxiliary variables (cf. Sec. 4.3).

III Formulate an Energy-Momentum conserving scheme based on the EL equations emanating from the new functional (cf. Sec. 4.4).

4.1 A New Variational Principle

Firstly, we want to propose a novel functional describing dynamical systems with primary and secondary constraints in Section 4.1.1, where we also derive the corresponding equations of motion. Next, we will show that those equations of motion inherit the Hamiltonian structure of the standard DAEs for constrained dynamics and can thus be derived from an augmented Hamiltonian (cf. Sec. 4.1.2). Eventually, the conservation of the symplectic structure and momentum maps will be demonstrated in Section 4.1.3.

4.1.1 Governing Equations

We introduce a new mixed functional for constrained mechanical systems, henceforth referred to as *GGL functional*, given by

$$\mathcal{S}(\mathbf{q}, \mathbf{v}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\gamma}) = \int_0^T \Big(L(\mathbf{q}, \mathbf{v}) - \boldsymbol{\lambda} \cdot \mathbf{g}(\mathbf{q}) + \mathbf{p} \cdot (\dot{\mathbf{q}} - \mathbf{v} - \mathbf{M}^{-1}\, \mathbf{G}(\mathbf{q})^{\mathrm{T}}\, \boldsymbol{\gamma}) \Big)\, \mathrm{d}t \ , \tag{4.1}$$

where $\mathbf{q}, \mathbf{v} \in \mathbb{R}^d$ denote the position and velocity, respectively. The Lagrange multipliers $\mathbf{p} \in \mathbb{R}^d$ enforces the kinematic relation and $\boldsymbol{\lambda}, \boldsymbol{\gamma} \in \mathbb{R}^m$ enforce the constraints on configuration level (3.2) and momentum level (3.15), respectively. For unconstrained systems the last equation boils down to Livens principle (2.18), where $\mathbf{p}$ enforces $\mathbf{v}$ to be the velocity vector of the system. As of before, $\mathbf{G}(\mathbf{q})$ denotes the gradient of the constraint function as defined in (3.3). The newly proposed action integral (4.1) differs from (3.12) as the constraints on momentum level (3.15) are enforced additionally. Hamilton's principle of least action given by the stationarity condition $\delta\mathcal{S} = 0$ with respect to every independent variable yields

$$\int_0^T \delta\mathbf{p} \cdot \left(\dot{\mathbf{q}} - \mathbf{v} - \mathbf{M}^{-1}\,\mathbf{G}(\mathbf{q})^{\mathrm{T}}\,\boldsymbol{\gamma})\right)\,\mathrm{d}t = 0\ , \tag{4.2a}$$

$$\int_0^T \left(\mathrm{D}_1 L(\mathbf{q},\mathbf{v}) \cdot \delta\mathbf{q} - \mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} \cdot \delta\mathbf{q} + \mathbf{p} \cdot \delta\dot{\mathbf{q}} - \mathbf{p} \cdot \mathbf{M}^{-1}\delta\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}\right)\,\mathrm{d}t = 0\ , \tag{4.2b}$$

$$\int_0^T \delta\mathbf{v} \cdot \left(\mathrm{D}_2 L(\mathbf{q},\mathbf{v}) - \mathbf{p}\right)\,\mathrm{d}t = 0\ , \tag{4.2c}$$

$$\int_0^T \delta\boldsymbol{\lambda} \cdot \mathbf{g}(\mathbf{q})\,\mathrm{d}t = 0\ , \tag{4.2d}$$

$$\int_0^T \mathbf{p} \cdot \mathbf{M}^{-1}\,\mathbf{G}(\mathbf{q})^{\mathrm{T}}\,\delta\boldsymbol{\gamma}\,\mathrm{d}t = 0\ . \tag{4.2e}$$

As one can see, relation (4.2b) requires some more effort in order to achieve the Euler-Langrange equation. Therefore, $\delta\dot{\mathbf{q}}$ can be replaced by making use of integration by parts as

$$\int_0^T \mathbf{p} \cdot \delta\dot{\mathbf{q}}\,\mathrm{d}t = -\int_0^T \delta\mathbf{q} \cdot \dot{\mathbf{p}}\,\mathrm{d}t + \delta\mathbf{q}(T) \cdot \mathbf{p}(T) - \delta\mathbf{q}(0) \cdot \mathbf{p}(0)\ . \tag{4.3}$$

The endpoint conditions (2.6) make the latter two terms vanish. Furthermore, the variation of the gradient of the constraint functions can be executed as

$$\delta\mathbf{G}(\mathbf{q}) = \mathrm{D}\mathbf{G}(\mathbf{q})\delta\mathbf{q} = \mathrm{D}^2\mathbf{g}(\mathbf{q})\delta\mathbf{q}\ . \tag{4.4}$$

In order to avoid the third order expression $\mathrm{D}^2\mathbf{g}(\mathbf{q})$, the stationarity condition (4.2b) can be written in terms of the individual constraint functions $g_{\mathrm{k}}(\mathbf{q})$ for $k = 1, ..., m$. Thus, the variation of the gradients is given by

$$\delta(\mathrm{D}g_k(\mathbf{q})) = \mathrm{D}^2 g_k(\mathbf{q})\delta\mathbf{q}\ , \tag{4.5}$$

where the constraint Hessian $\mathrm{D}^2 g_k(\mathbf{q}) \in \mathbb{R}^{d\times d}$. Consequently, the arbitrariness of the variations $\delta\mathbf{q}$, $\delta\mathbf{v}$, $\delta\mathbf{p}$, $\delta\boldsymbol{\lambda}$ and $\delta\boldsymbol{\gamma}$ can be taken into account such that the governing

DAEs are deduced as

$$\dot{\mathbf{q}} = \mathbf{v} + \mathbf{M}^{-1}\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma} \ , \tag{4.6a}$$

$$\dot{\mathbf{p}} = \mathrm{D}_1 L(\mathbf{q}, \mathbf{v}) - \mathbf{M}^{-1}\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} - \sum_{k=1}^{m} \gamma_k \mathrm{D}^2 g_k(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} \ , \tag{4.6b}$$

$$\mathbf{p} = \mathrm{D}_2 L(\mathbf{q}, \mathbf{v}) \ , \tag{4.6c}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{q}) \ , \tag{4.6d}$$

$$\mathbf{0} = \mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} \ . \tag{4.6e}$$

Note that (4.6c) represents the fiber derivative of the newly proposed variational principle, such that the Lagrange multiplier $\mathbf{p}$ denotes the conjugate momenta. By introducing the secondary constraint to the functional, the emanating Euler-Lagrange equations are DAEs with index $\nu = 2$, similarly to GGL stabilized equations of motion, whereas the standard DAEs of constrained dynamics have index $\nu = 3$. Thus, the newly achieved DAEs can be regarded as an extension to the classical GGL stabilization. However, the third term in (4.6b) is of crucial importance as it provides a Hamiltonian structure of equations of motion, in contrast to the classical GGL method. This Hamiltonian structure can be carried over to corresponding variational integration schemes.

Note that similarly to the original GGL stabilization (cf. Sec. 3.2.3), we can show that the Lagrangian multiplies $\boldsymbol{\gamma}$ vanish in the time-continuous case. In analogy to the procedure from (3.39) to (3.41), we insert the kinematic equation (4.6a) into the constraint on momentum level (4.6e), make use of the time-derivative of the primary constraint (4.6d) and eventually obtain

$$\mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{G}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma} = \mathbf{0} \ , \tag{4.7}$$

where $\mathbf{G}(\mathbf{q})\mathbf{M}^{-1}\mathbf{G}(\mathbf{q})^{\mathrm{T}}$ is non-singular by assumption. Consequently, $\boldsymbol{\gamma} = \mathbf{0}$ during the whole motion, because the secondary constraints are fulfilled a priori. However, this is not the case within discrete frameworks later on. Thus, Lagrangian multipliers will not vanish as they need to enforce the secondary constraints in a discrete sense.

4.1.2 Hamiltonian Structure

An augmented Hamiltonian for the constrained system reads

$$\mathcal{H}_{\lambda\gamma}(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p}) + \boldsymbol{\lambda} \cdot \mathbf{g}^{\mathbf{q}}(\mathbf{q}) + \boldsymbol{\gamma} \cdot \mathbf{g}^{\mathbf{v}}(\mathbf{q}, \mathbf{p}) \ , \tag{4.8}$$

where $H(\mathbf{q}, \mathbf{p})$ denotes the Hamiltonian function of the unconstrained natural system (2.15). In the last equation we have introduced the distinct functions $\mathbf{g}^{\mathbf{q}}(\mathbf{q}) = \mathbf{g}(\mathbf{q})$ for the holonomic constraint on configuration level and $\mathbf{g}^{\mathbf{v}}(\mathbf{q}, \mathbf{p}) = \mathrm{D}\mathbf{g}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}$ for the corresponding constraint on momentum level. We can show that the EL equations of the GGL functional (4.6) can be traced back to the augmented Hamiltonian (4.8). Thus,

differentiation of (4.8) with respect to all single variables yields

$$\mathrm{D}_2\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) = \mathrm{D}_2 H(\mathbf{q},\mathbf{p}) + \mathrm{D}_2\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})^{\mathrm{T}}\boldsymbol{\gamma} \;, \tag{4.9a}$$
$$\mathrm{D}_1\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) = \mathrm{D}_1 H(\mathbf{q},\mathbf{p}) + \mathrm{D}\mathbf{g}^{\mathbf{q}}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} + \mathrm{D}_1\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})^{\mathrm{T}}\boldsymbol{\gamma} \;, \tag{4.9b}$$
$$\mathrm{D}_{\boldsymbol{\lambda}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) = \mathbf{g}^{\mathbf{q}}(\mathbf{q}) \;, \tag{4.9c}$$
$$\mathrm{D}_{\boldsymbol{\gamma}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) = \mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p}) \;, \tag{4.9d}$$

which can be related to the Euler-Lagrange equations of the GGL functional after elimination of the velocities by employing the Legendre transformation (4.6c). Thus, we obtain

$$\dot{\mathbf{q}} = +\mathrm{D}_2\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) \;, \tag{4.10a}$$
$$\dot{\mathbf{p}} = -\mathrm{D}_1\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) \;, \tag{4.10b}$$
$$\mathbf{0} = +\mathrm{D}_{\boldsymbol{\lambda}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) \;, \tag{4.10c}$$
$$\mathbf{0} = +\mathrm{D}_{\boldsymbol{\gamma}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) \;, \tag{4.10d}$$

where the first two differential equations can be recast in the known abstract fashion similar to (2.27) as

$$\dot{\mathbf{z}} = \mathbb{J}\mathrm{D}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{z}) \;, \tag{4.11}$$

where the canonical structure matrix $\mathbb{J}$ from (2.28) is used. Next, we want to show that the equations of motion of the novel framework conserve the Hamiltonian exactly. For that purpose, we follow the procedure for unconstrained dynamics (2.17) and compute the time derivative of the augmented Hamiltonian (4.8) such that

$$\begin{aligned}\dot{\mathcal{H}}_{\boldsymbol{\lambda\gamma}} &= \mathrm{D}_1\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p})\cdot\dot{\mathbf{q}} + \mathrm{D}_2\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p})\cdot\dot{\mathbf{p}} + \mathrm{D}_{\boldsymbol{\lambda}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p})\cdot\dot{\boldsymbol{\lambda}} + \mathrm{D}_{\boldsymbol{\gamma}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p})\cdot\dot{\boldsymbol{\gamma}} \\ &= \mathrm{D}_1\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p})\cdot\mathrm{D}_2\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) - \mathrm{D}_2\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p})\cdot\mathrm{D}_1\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q},\mathbf{p}) + \mathbf{0}\cdot\dot{\boldsymbol{\lambda}} + \mathbf{0}\cdot\dot{\boldsymbol{\gamma}} \\ &= 0 \;,\end{aligned} \tag{4.12}$$

where the Hamiltonian equations of motion (4.10) have been considered. As the augmented Hamiltonian (4.8) is conserved along solutions of the equations of motion also the Hamiltonian H itself is conserved since both constraints on configuration level and momentum level are identically zero such that $\dot{H} = 0$. In contrast to the originial GGL formulation [50] (cf. Sec. 3.2.3), this conservation law holds regardless of the actual value of the Lagrange multipliers $\boldsymbol{\gamma}$.

4.1.3 Symplectic Structure and Momentum Map Conservation

As for the standard DAEs of constrained dynamics (cf. Sec. 3.1.3), we can show that the GGL functional inherits the symplectic structure of Hamiltonian systems and thus the symplectic two-form is conserved along solutions of (4.10). We begin by deriving the

total differentials based on the equations of motion as

$$\mathrm{d}\dot{\mathbf{q}} = \mathrm{D}_{21}^2 H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} + \mathrm{D}_{22}^2 H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p} + \mathrm{d}\left(\mathrm{D}_2\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})^{\mathrm{T}}\boldsymbol{\gamma}\right) , \tag{4.13a}$$

$$\mathrm{d}\dot{\mathbf{p}} = -\mathrm{D}_{11}^2 H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} - \mathrm{D}_{12}^2 H(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p} - \mathrm{d}\left(\mathrm{D}\mathbf{g}^{\mathbf{q}}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\right) - \mathrm{d}\left(\mathrm{D}_1\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})^{\mathrm{T}}\boldsymbol{\gamma}\right) , \tag{4.13b}$$

$$\mathbf{0} = \mathrm{D}\mathbf{g}^{\mathbf{q}}(\mathbf{q})\,\mathrm{d}\mathbf{q} , \tag{4.13c}$$

$$\mathbf{0} = \mathrm{D}_1\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} + \mathrm{D}_2\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p} . \tag{4.13d}$$

Once more it is straightforward to compute the temporal evolution of Ω by means of the product rule (2.88) such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega = \mathrm{d}\dot{\mathbf{q}} \wedge \mathrm{d}\mathbf{p} + \mathrm{d}\mathbf{q} \wedge \mathrm{d}\dot{\mathbf{p}} , \tag{4.14}$$

where the above differential equations (4.13a) and (4.13b) can be inserted. In analogy to Section 3.1.3 one can consider the symmetry of the Hessian of H and make use of the properties of the wedge product. Therefore, all terms cancel out except for those emanating from the constraint on momentum level $\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})$. We therefore obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Omega &= \mathrm{d}\left(\mathrm{D}_2\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})^{\mathrm{T}}\boldsymbol{\gamma}\right) \wedge \mathrm{d}\mathbf{p} - \mathrm{d}\mathbf{q} \wedge \mathrm{d}\left(\mathrm{D}_1\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})^{\mathrm{T}}\boldsymbol{\gamma}\right) \\
&= \mathrm{D}_2\mathbf{g}^{\mathbf{v}\mathrm{T}}\,\mathrm{d}\boldsymbol{\gamma} \wedge \mathrm{d}\mathbf{p} + \mathrm{D}_1\mathbf{g}^{\mathbf{v}\mathrm{T}}\,\mathrm{d}\boldsymbol{\gamma} \wedge \mathrm{d}\mathbf{q} + \sum_{k=1}^{m} \gamma_k \mathrm{D}_{12}^2 g_k^{\mathbf{v}}\,\mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} + \sum_{k=1}^{m} \gamma_k \mathrm{D}_{21}^2 g_k^{\mathbf{v}}\,\mathrm{d}\mathbf{p} \wedge \mathrm{d}\mathbf{q} \\
&= \mathrm{d}\boldsymbol{\gamma} \wedge (\mathrm{D}_1\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q} + \mathrm{D}_2\mathbf{g}^{\mathbf{v}}(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{p}) + \sum_{k=1}^{m} \gamma_k \left(\mathrm{D}_{12}^2 g_k^{\mathbf{v}} - (\mathrm{D}_{21}^2 g_k^{\mathbf{v}})^{\mathrm{T}}\right) \mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p} \\
&= 0 ,
\end{aligned} \tag{4.15}$$

where the first term vanishes in view of the total differential of the secondary constraint (4.13d) and the second one cancels due to the symmetry of the Hessian of $g_k^{\mathbf{v}}$. Eventually, we are able to proof the symplecticness of the equations of motion induced by the GGL functional. Again this property does not depend on the Lagrange multiplier $\boldsymbol{\gamma}$, which is an advantage over the original GGL method by Gear et al. [50], for which $\boldsymbol{\gamma} = \mathbf{0}$ was required in order to conserve Ω (cf. Sec. 3.2.3).

Moreover, it can be demonstrated that the constrained dynamics described with the GGL functional preserve the momentum maps $\mathbf{J}$ of the system defined in (2.40). For that purpose, we assume that the augmented Hamiltonian (4.8) is G-invariant in the sense of (2.37). Consequently, one can consider the infinitesimal generator (2.38) to obtain

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathcal{H}_{\boldsymbol{\lambda}\boldsymbol{\gamma}}(\boldsymbol{\Phi}(\mathbf{g}(\alpha),\mathbf{z}))\Big|_{\alpha=0} = \mathrm{D}\mathcal{H}_{\boldsymbol{\lambda}\boldsymbol{\gamma}}(\mathbf{z}) \cdot \boldsymbol{\xi}_p = 0 , \tag{4.16}$$

which represents an augmentation of the original orthogonality condition (2.39). In the next step, we proceed analogously to (2.41) and compute the time derivative of the

projection of the momentum map, viz.

$$\frac{\mathrm{d}}{\mathrm{d}t} J_{\boldsymbol{\xi}}(\mathbf{z}) = \mathrm{D}J_{\boldsymbol{\xi}}(\mathbf{z}) \cdot \dot{\mathbf{z}} = \mathrm{D}\mathcal{H}_{\boldsymbol{\lambda}\boldsymbol{\gamma}}(\mathbf{z}) \cdot \mathbb{J}^{\mathrm{T}} \mathbb{J}^{-1} \boldsymbol{\xi}_P(\mathbf{z}) = -\mathrm{D}\mathcal{H}_{\boldsymbol{\lambda}\boldsymbol{\gamma}}(\mathbf{z}) \cdot \boldsymbol{\xi}_P(\mathbf{z}) \ . \tag{4.17}$$

Note that we have replaced the time derivative of the phase space vector with the abstract Hamiltonian equations (4.11) for the augmented system. Considering the recently derived condition (4.16), we can eventually state the conservation of momentum maps

$$\frac{\mathrm{d}}{\mathrm{d}t} J_{\boldsymbol{\xi}}(\mathbf{z}) = \frac{\mathrm{d}}{\mathrm{d}t} \left(\mathbf{J}(\mathbf{z}) \cdot \boldsymbol{\xi} \right) = 0 \ , \tag{4.18}$$

if the Hamiltonian is G-invariant under a certain action $\boldsymbol{\Phi}$ corresponding to $\boldsymbol{\xi} \in \mathcal{TG}$. For a more detailled introduction recall Sec. 2.2.3.

4.2 GGL Variational Integrator

In this section we will straightforwardly discretize the new variational principle from Section 4.1 and derive a simple time integration scheme in Section 4.2.1. Subsequently, discrete conservation principles for that method are explored in Section 4.2.2. Lastly, the performance by means of a numerical example will be investigated in Section 4.2.3.

4.2.1 Governing Equations

Let us construct a time-stepping scheme by means of a direct discretization of the GGL functional (4.1). Enforcing the constraints on configuration and momentum level in the endpoint and discretizing the velocity by means of an explicit Euler method, we obtain the discrete action integral

$$\begin{aligned} \mathcal{S}_{\mathrm{d}} = \sum_{n=0}^{N-1} \Big[& h\, L(\mathbf{q}^n, \mathbf{v}^n) - h\, \boldsymbol{\lambda}^{n+1} \cdot \mathbf{g}(\mathbf{q}^{n+1}) \\ & + \mathbf{p}^{n+1} \cdot \left(\mathbf{q}^{n+1} - \mathbf{q}^n - h\, \mathbf{v}^n - h\, \mathbf{M}^{-1} \mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}} \boldsymbol{\gamma}^{n+1} \right) \Big] \qquad (4.19) \\ & + \mathbf{p}^0 \cdot (\mathbf{q}^0 - \bar{\mathbf{q}}) - h\, \boldsymbol{\lambda}^0 \cdot \mathbf{g}(\mathbf{q}^0) \ . \qquad (4.20) \end{aligned}$$

It is noted that additional Lagrange multiplier $\mathbf{p}^0$ enforce the initial configuration and $\boldsymbol{\lambda}^0$ demand the satisfaction of the primary constraints in the initial state. This approach facilitates the subsequent procedure of deriving the equations of motion. Note that this discrete action integral is a direct enhancement of the constrained symplectic Euler B method (3.46) with respect to the constraint on momentum level. Stationarity conditions can be applied directly to the discrete functional, yielding

$$\sum_{n=0}^{N-1} \delta \mathbf{p}^{n+1} \cdot \left(\mathbf{q}^{n+1} - \mathbf{q}^n - h\, \mathbf{v}^n - h\, \mathbf{M}^{-1} \mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}} \boldsymbol{\gamma}^{n+1} \right) = 0 \ , \tag{4.21a}$$

$$\sum_{n=0}^{N-1} \delta\mathbf{q}^n \cdot \Big(h\, \mathrm{D}_1 L(\mathbf{q}^n, \mathbf{v}^n) - \mathbf{p}^{n+1} \Big) + \delta\mathbf{q}^0 \cdot \mathbf{p}^0 \tag{4.21b}$$

$$+ \sum_{n=0}^{N-1} \delta\mathbf{q}^{n+1} \cdot \left(-h\, \mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}} \boldsymbol{\lambda}^{n+1} + \mathbf{p}^{n+1} - h \sum_{k=1}^{m} \gamma_k^{n+1} \mathrm{D}^2 g_k(\mathbf{q}^{n+1}) \mathbf{M}^{-1} \mathbf{p}^{n+1} \right) = 0 \ ,$$

$$\sum_{n=0}^{N-1} \delta\mathbf{v}^n \cdot \Big(h\, \mathrm{D}_2 L(\mathbf{q}^n, \mathbf{v}^n) - h\, \mathbf{p}^{n+1} \Big) = 0 \ , \tag{4.21c}$$

$$\sum_{n=0}^{N-1} \delta\boldsymbol{\lambda}^{n+1} \cdot \mathbf{g}(\mathbf{q}^{n+1}) = 0 \ , \tag{4.21d}$$

$$\sum_{n=0}^{N-1} \delta\boldsymbol{\gamma}^{n+1} \cdot \mathbf{G}(\mathbf{q}^{n+1}) \mathbf{M}^{-1} \mathbf{p}^{n+1} = 0 \ . \tag{4.21e}$$

Applying an index-shift in the second part of (4.21b) from $n+1$ to n and taking into account the arbitrariness of all variations, we can write the discrete EL equations

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{v}^n + h\, \mathbf{M}^{-1} \mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}} \boldsymbol{\gamma}^{n+1} \ , \tag{4.22a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = h\, \mathrm{D}_1 L(\mathbf{q}^n, \mathbf{v}^n) - h\, \mathbf{G}(\mathbf{q}^n)^{\mathrm{T}} \boldsymbol{\lambda}^n - h \sum_{k=1}^{m} \gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^n) \mathbf{M}^{-1} \mathbf{p}^n \ , \tag{4.22b}$$

$$\mathbf{p}^{n+1} = \mathrm{D}_2 L(\mathbf{q}^n, \mathbf{v}^n) \ , \tag{4.22c}$$

$$\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{0} \ , \tag{4.22d}$$

$$\mathbf{G}(\mathbf{q}^{n+1}) \mathbf{M}^{-1} \mathbf{p}^{n+1} = \mathbf{0} \ . \tag{4.22e}$$

for $n = 0, ..., N-1$. In total we have obtained a set of $(3\,d + 2\,m)$ equations for the unknowns $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}, \mathbf{v}^n, \boldsymbol{\lambda}^n, \boldsymbol{\gamma}^{n+1})$ in every time step. These are discrete counterparts of the continuous EL equations given in (4.6). It is advantageous that, due to the enhancement of the discrete action integral, the secondary constraints are now directly enforced at the endpoint (cf. relation (4.22e). With respect to the equations of motion given by the constrained symplectic Euler B scheme (3.47), we furthermore obtain two additional terms in the configuration and momentum equations. The present integrator thus generalizes the constrained symplectic Euler method. As of before, relation (4.22c) can be interpreted as the discrete fiber derivative of the Legendre transformation, which links velocity and momentum quantities.

4.2.2 Conservation Properties

It is clear that the constraints are correctly captured in every time step by design (see relations (4.22d) and (4.22e)). Thus, the present integration scheme conserves the constrained phase space (3.16) in a discrete sense. One might have anticipated that the present scheme inherits the Hamiltonian structure of the DAEs emanating from the GGL functional. However, this scheme does actually not inherit the conservation properties of the time-continuous EL equations. The total energy particularly can only be

conserved if gradients fulfill certain conditions. This is in general not the case and requires more sophisticated gradient modifications as will be shown in Section 4.4 dealing with EM schemes based on the newly proposed GGL functional. Moreover, we can show that the integrator governed by (4.22) is not symplectic. In order to demonstrate that, we derive the differentials of (4.22a) and (4.22b) after having substituted (4.22c). This yields

$$\mathrm{d}\mathbf{q}^{n+1} - \mathrm{d}\mathbf{q}^{n} = h\,\mathbf{M}^{-1}\,\mathrm{d}\mathbf{p}^{n+1} + h\,\mathrm{d}(\mathbf{M}^{-1}\mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}}\boldsymbol{\gamma}^{n+1})\;, \tag{4.23a}$$

$$\mathrm{d}\mathbf{p}^{n+1} - \mathrm{d}\mathbf{p}^{n} = h\,\mathrm{D}_{11}^{2}L(\mathbf{q}^{n},\mathbf{v}^{n})\,\mathrm{d}\mathbf{q}^{n} - h\,\mathrm{d}(\mathbf{G}(\mathbf{q}^{n})^{\mathrm{T}}\boldsymbol{\lambda}^{n}) - h\,\mathrm{d}(\sum_{k=1}^{m}\gamma_{k}^{n}\mathrm{D}^{2}g_{k}(\mathbf{q}^{n})\mathbf{M}^{-1}\mathbf{p}^{n})\;. \tag{4.23b}$$

Note that $\mathrm{D}_{12}^{2}L(\mathbf{q}^{n},\mathbf{v}^{n}) = \mathbf{0}$ is valid by assumption. The differential forms of the constraint equations for $\mathbf{g}^{\mathbf{q}}$ in (4.22d) and for $\mathbf{g}^{\mathbf{v}}$ in (4.22e) read

$$\mathrm{d}\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{G}(\mathbf{q}^{n+1})\,\mathrm{d}\mathbf{q}^{n+1} = \mathbf{0}\;, \tag{4.24a}$$

$$\mathrm{d}\mathbf{g}_{v}(\mathbf{q}^{n+1},\mathbf{p}^{n+1}) = \mathrm{D}_{\mathbf{q}}\mathbf{g}_{v}\,\mathrm{d}\mathbf{q}^{n+1} + \mathrm{D}_{\mathbf{p}}\mathbf{g}_{v}\,\mathrm{d}\mathbf{p}^{n+1} = \mathbf{0}\;. \tag{4.24b}$$

Following the argumentation as shown by Leimkuhler et al. [12], we can show that the following relationship holds:

$$\mathrm{d}\mathbf{q}^{n}\wedge\mathrm{d}(\mathbf{G}^{n\mathrm{T}}\boldsymbol{\lambda}^{n}) = \mathrm{d}\mathbf{q}^{n}\wedge\mathbf{G}^{n\mathrm{T}}\,\mathrm{d}\boldsymbol{\lambda}^{n} + \mathrm{d}\mathbf{q}^{n}\wedge\sum_{k=1}^{m}\lambda_{k}^{n}\mathrm{D}^{2}g_{k}^{n}\,\mathrm{d}\mathbf{q}^{n} = \mathbf{0}\;. \tag{4.25}$$

By making use of the matrix multiplication property of the wedge product (A.15) in the first term and substituting (4.24a), the first term vanishes. For the second term one can take account of the symmetry of the Hessian of the constraint on configuration level. Therefore, also this wedge product vanishes according to Section 2.3.3. Making use of the skew-symmetry of the wedge product (A.13), one can deduce that

$$\mathrm{d}\mathbf{p}^{n+1}\wedge(\,\mathrm{d}\mathbf{q}^{n+1} - \mathrm{d}\mathbf{q}^{n}) + (\,\mathrm{d}\mathbf{p}^{n+1} - \mathrm{d}\mathbf{p}^{n})\wedge\mathrm{d}\mathbf{q}^{n} = \mathrm{d}\mathbf{q}^{n}\wedge\mathrm{d}\mathbf{p}^{n} - \mathrm{d}\mathbf{q}^{n+1}\wedge\mathrm{d}\mathbf{p}^{n+1}\;. \tag{4.26}$$

If we plug in the previously derived differential equations, we obtain

$$\begin{aligned}\mathrm{d}\mathbf{q}^{n}\wedge\mathrm{d}\mathbf{p}^{n} - \mathrm{d}\mathbf{q}^{n+1}\wedge\mathrm{d}\mathbf{p}^{n+1} = {}& \\ & \mathrm{d}\mathbf{p}^{n+1}\wedge h\,\mathbf{M}^{-1}\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{p}^{n+1}\wedge\mathrm{d}(\mathrm{D}_{\mathbf{p}}\mathbf{g}^{\mathbf{v}}(\mathbf{q}^{n+1},\mathbf{p}^{n+1})^{\mathrm{T}}\boldsymbol{\gamma}^{n+1}) \\ & + h\,\mathrm{D}_{11}^{2}L(\mathbf{q}^{n},\mathbf{v}^{n})\,\mathrm{d}\mathbf{q}^{n}\wedge\mathrm{d}\mathbf{q}^{n} + \mathrm{d}\mathbf{q}^{n}\wedge h\,\mathrm{d}(\mathbf{G}(\mathbf{q}^{n})^{\mathrm{T}}\boldsymbol{\lambda}^{n}) \\ & - h\,\mathrm{d}(\sum_{k=1}^{m}\gamma_{k}^{n}\mathrm{D}_{\mathbf{q}}\mathbf{g}_{k}^{v}(\mathbf{q}^{n},\mathbf{p}^{n}))\wedge\mathrm{d}\mathbf{q}^{n}\;.\end{aligned} \tag{4.27}$$

Once more we can employ the properties of the wedge product to get rid of the first and third term. The fourth one can be canceled out due to the relation (4.25). Executing

the differentials, we obtain

$$\begin{aligned}
&\mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n - \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} = \\
&\quad \mathrm{D}_{\mathbf{p}}\mathbf{g}^{\mathrm{v}}(\mathbf{q}^{n+1}, \mathbf{p}^{n+1})^{\mathrm{T}}\, \mathrm{d}\mathbf{p}^{n+1} \wedge h\, \mathrm{d}\boldsymbol{\gamma}^{n+1} + \mathrm{D}_{\mathbf{q}}\mathbf{g}^{\mathrm{v}}(\mathbf{q}^{n}, \mathbf{p}^{n})^{\mathrm{T}}\, \mathrm{d}\mathbf{q}^{n} \wedge h\, \mathrm{d}\boldsymbol{\gamma}^{n} \\
&\quad + \mathrm{d}\mathbf{p}^{n+1} \wedge \sum_{k=1}^{m} \gamma_k^{n+1} \mathrm{D}_{21}^2 g_v^k(\mathbf{q}^{n+1}, \mathbf{p}^{n+1})\, \mathrm{d}\mathbf{q}^{n+1} - \mathrm{d}\mathbf{p}^{n} \wedge \sum_{k=1}^{m} \gamma_k^{n} (\mathrm{D}_{12}^2 g_v^k(\mathbf{q}^{n}, \mathbf{p}^{n}))^{\mathrm{T}}\, \mathrm{d}\mathbf{q}^{n} \ .
\end{aligned} \tag{4.28}$$

Generally, this expression does not vanish since the quantities are evaluated at different points in time. However, taking the limit $h \to 0$, the scheme tends to symplecticness since $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}, \boldsymbol{\gamma}^{n+1}) \to (\mathbf{q}^{n}, \mathbf{p}^{n}, \boldsymbol{\gamma}^{n})$. In the limit the total differentials of the constraint on momentum level (4.24b) and the symmetry of the Hessian matrices can be considered such that

$$\lim_{h \to 0} \left(\mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n - \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} \right) = 0 \ . \tag{4.29}$$

Eventually we must state, that the given integration scheme is not symplectic. In Section 4.3 we will show that other choices of discretization of the action integral will lead to integrators that are actually symplectic. But first, we want to demonstrate the current integrator's properties by means of a numerical example.

4.2.3 Numerical Example: Mathematical Pendulum

As a dynamical system the mathematical pendulum shall be investigated for a total simulation time of $T = 10\,\mathrm{s}$ which is divided into subintervals with time step size $h = 0.05\,\mathrm{s}$. Gravitation acts in the $\mathbf{e}_3$-direction according to an acceleration vector

$$\mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ -9.81 \end{bmatrix} \mathrm{m/s^2} \ . \tag{4.30}$$

The pendulum, which is displayed in Fig. 4.1 and whose length is $l = 1\,\mathrm{m}$, underlies the constraint on configuration level

$$g^{\mathrm{q}}(\mathbf{q}) = \frac{1}{2} \left(\mathbf{q} \cdot \mathbf{q} - l^2 \right) = 0 \tag{4.31}$$

and on momentum level

$$g^{\mathrm{v}}(\mathbf{q}, \mathbf{p}) = \mathbf{G}(\mathbf{q}) \cdot \mathbf{M}^{-1}\mathbf{p} = \frac{1}{m}\, \mathbf{q} \cdot \mathbf{p} = 0 \ . \tag{4.32}$$

The pendulum is initially released at $\mathbf{q}(t = 0) = \mathbf{q}^0 = [1\,,\, 0\,,\, 0]^{\mathrm{T}}\,\mathrm{m}$ with a velocity $\mathbf{v}(t = 0) = \mathbf{v}^0 = [0\,,\, 1\,,\, 0]^{\mathrm{T}}\,\mathrm{m/s}$. The point mass has a total mass of $m = 1\,\mathrm{kg}$ and the DEL (4.22) are solved with Newton's method in every time step. The corresponding tolerance is set to $\varepsilon_{\mathrm{tol}} = 10^{-9}$. The computation has been performed using the *metis* code, which is available at [58].

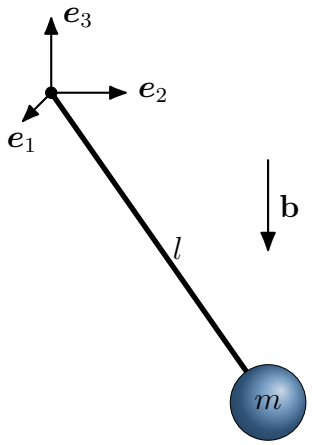

Figure 4.1: Mathematical Pendulum

Firstly, we can verify that the constraints both on configuration (cf. Fig. 4.2) and momentum level (cf. Fig. 4.3) are correctly captured down to machine precision. In Fig. 4.4 we can observe that the total energy oscillates largely but remains stable also for long time simulations, if h is chosen sufficiently small. The increments in the Hamiltonian H from one time step to another, as it is depicted in Fig. 4.6 is of the same order of magnitude as H itself. Fig. 4.5 shows that the present integrator does not preserve the angular momentum. However, the oscillations in angular momentum around the symmetry axis (see Fig. 4.7) are comparably small and therefore bodes well for a high accuracy of the simulation method. Note that Fig. 4.6 and Fig. 4.7 which show the increments of H and L_3 also display the respective standard deviations, which are defined in (A.11) and rely on the mean value (A.12).

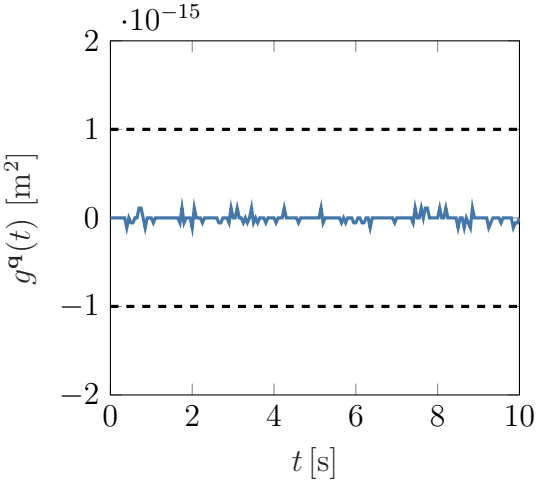

Figure 4.2: Constraints on configuration level

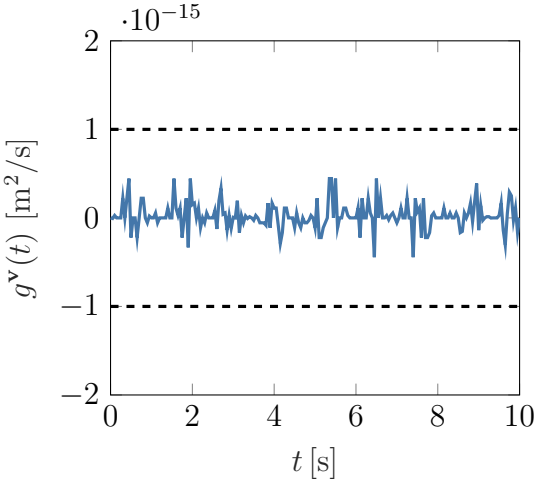

Figure 4.3: Constraints on velocity level

In Fig. 4.8 it becomes visible that the present variational integrator ("GGL-VI") is first-order accurate just like the constrained symplectic Euler B scheme ("CSE-B") presented in Section 3.3.2 and a method with classical GGL stabilization (cf. Sec. 3.3.3). In a double logarithmic diagram we have displayed the relative error in the positions after one second $\mathbf{q}(t = 1\,\mathrm{s})$ for multiple choices of the time step size h. The relative error is

defined via

$$e = \frac{||\mathbf{q}(t = 1\,\mathrm{s}) - \mathbf{q}_{\mathrm{ref}}||}{||\mathbf{q}_{\mathrm{ref}}||} \,, \tag{4.33}$$

where $\mathbf{q}_{\mathrm{ref}}$ represents the solution of the newly derived variational integrator with $h = 10^{-4}\,\mathrm{s}$. Moreover, one can observe that the classical GGL stabilization induces a larger error when enforcing the secondary constraint. The newly proposed GGL variational integrator is capable of enforcing the constraint on momentum level (cf. Fig. 4.3), thus conserving the constraint phase space $\mathcal{P}_{\mathrm{c}}$, while maintaining the same approximation accuracy as the symplectic Euler scheme (cf. Fig. 4.8).

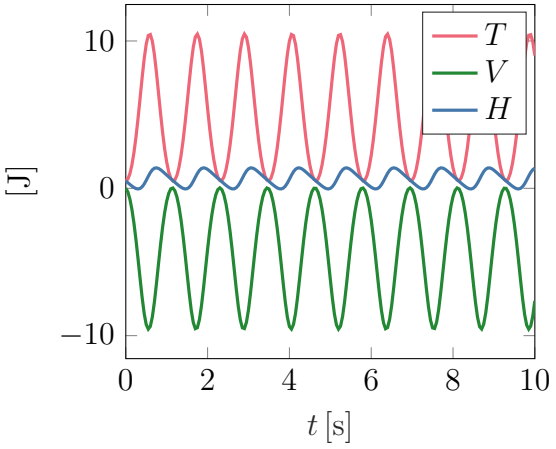

Figure 4.4: Energy quantities

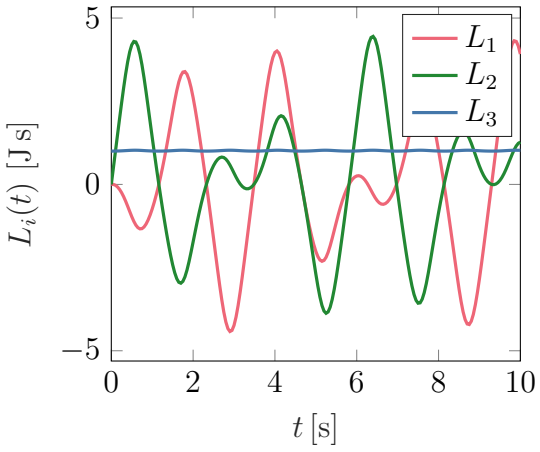

Figure 4.5: Angular momentum

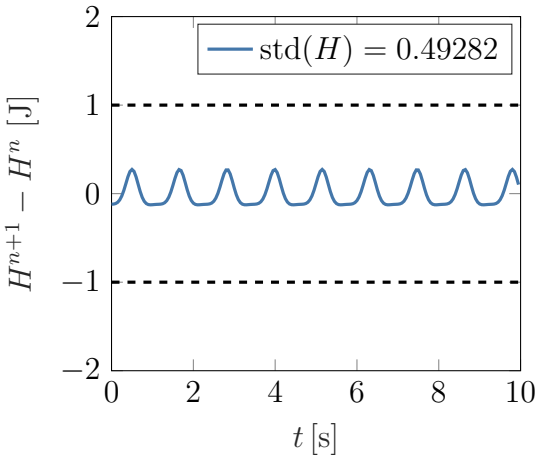

Figure 4.6: Hamiltonian difference

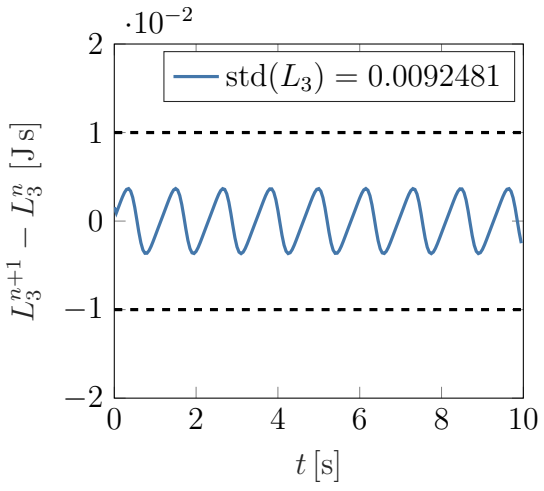

Figure 4.7: Angular momentum difference

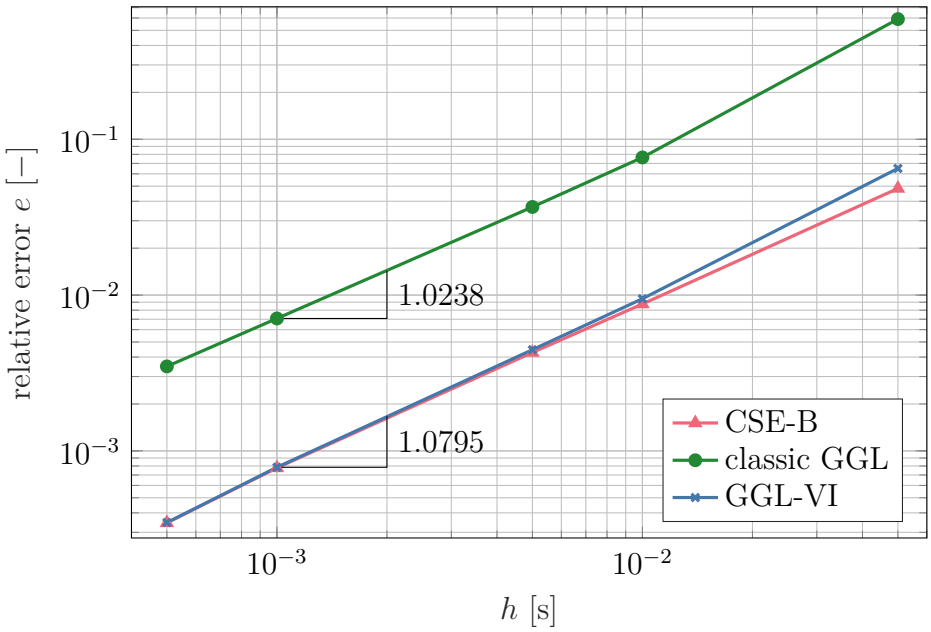

Figure 4.8: h-convergence of relative error in $\mathbf{q}$

4.3 Symplectic One-stage Methods

Since we could not capture the symplectic structure of the GGL functional and its DEL with our first discretization, as shown in the previous section, we will now explore a more complex ansatz, giving the basic idea in Section 4.3.1. After demonstrating that the emanating integration schemes are symplectic in Section 4.3.2, more detailed governing equations will be derived in Section 4.3.3. Furthermore, two different approximations of the primary constraints will be discussed in Section 4.3.4. In the last part of this section, we will investigate the motion of a rigid gyroscopic top numerically, making use of the newly derived integration schemes (cf. Sec. 4.3.5).

4.3.1 Basic Structure and Discrete Action Integral

Inspired by the one-stage theta method for optimally controlled systems by Betsch et al. [25], we can demonstrate a more sophisticated approximation of the action integral by introducing further auxiliary variables in the following fashion:

$$\mathcal{S}_\mathrm{d} = \sum_{n=0}^{N-1} \Big[L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) + \mathbf{p}^{n+1} \cdot \Big(\mathbf{q}^{n+1} - \mathbf{q}^n - \mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) \Big) + \mathbf{P}^n \cdot \Big(\mathbf{Q}^n \quad - \mathbf{q}^n - \mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) \Big) \Big] . \tag{4.34}$$

In this principle $L_\mathrm{d}^{\boldsymbol{\lambda}}$ represents a discrete version of the augmented Lagrangian for constrained mechanical systems (3.8) such that

$$L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) \approx \int_{t^n}^{t^{n+1}} \left[L(\mathbf{q}, \mathbf{v}) - \boldsymbol{\lambda} \cdot \mathbf{g}(\mathbf{q})\right] \mathrm{d}t \ , \tag{4.35}$$

whereas $\mathbf{f}_\mathrm{d}^\gamma$ denotes the right hand side vector of the discrete kinematic equation corresponding to (4.6a), such that $\dot{\mathbf{q}} = \mathbf{f}^\gamma(\mathbf{q}, \mathbf{v})$. Auxiliary position vectors $\mathbf{Q}^n$ and momenta $\mathbf{P}^n$ have been introduced. For some cases, those auxiliary quantities can be condensed in every time-step. Their purpose is to simplify the derivations of the DEL and the proofs of conservation properties. Note that this discrete action integral (4.34) once more takes account of constraints both on configuration and momentum level. Discrete versions of the constraints, being enforced by Lagrange multiplier $\boldsymbol{\lambda}^n$ and $\boldsymbol{\gamma}^n$, are part of $L_\mathrm{d}^{\boldsymbol{\lambda}}$ and $\mathbf{f}_\mathrm{d}^\gamma$, respectively.

Evaluating the discrete stationarity conditions, we deduce that

$$\sum_{n=0}^{N-1} \delta\mathbf{p}^{n+1} \cdot \left[\mathbf{q}^{n+1} - \mathbf{q}^n - \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})\right] = 0 \ , \tag{4.36a}$$

$$\sum_{n=0}^{N-1} \delta\mathbf{P}^{n} \cdot \left[\mathbf{Q}^n \ \ - \mathbf{q}^n - \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})\right] = 0 \ , \tag{4.36b}$$

$$\begin{aligned}\sum_{n=0}^{N-1} \delta\mathbf{q}^{n} \cdot \Big[&\mathrm{D}_1 L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) - \mathbf{p}^{n+1} - \mathrm{D}_1 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right)\Big] \\ &+ \sum_{n=0}^{N-1} \delta\mathbf{q}^{n+1} \cdot \mathbf{p}^{n+1} = 0 \ ,\end{aligned} \tag{4.36c}$$

$$\sum_{n=0}^{N-1} \delta\mathbf{Q}^{n} \cdot \left[\mathrm{D}_2 L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) + \mathbf{P}^n - \mathrm{D}_2 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right)\right] = 0 \ , \tag{4.36d}$$

$$\sum_{n=0}^{N-1} \delta\mathbf{v}^{n+1} \cdot \left[\mathrm{D}_3 L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) - \mathrm{D}_3 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right)\right] = 0 \ , \tag{4.36e}$$

$$\sum_{n=0}^{N-1} \delta\boldsymbol{\lambda}^{n} \cdot \mathrm{D}_{\boldsymbol{\lambda}} L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1}) = 0 \ , \tag{4.36f}$$

$$\sum_{n=0}^{N-1} \delta\boldsymbol{\gamma}^{n} \cdot \mathrm{D}_{\gamma} \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) = 0 \ . \tag{4.36g}$$

Firstly, it can be easily seen that stationarity conditions with respect to momentum quantities (4.36a) and (4.36b) lead to the fact that the auxiliary position vector simply denotes the configuration at t^{n+1}, viz.

$$\mathbf{Q}^n = \mathbf{q}^{n+1} \ . \tag{4.37}$$

In the stationarity condition with respect to $\mathbf{q}$ in (4.36c) an index shift in the second sum from $n+1$ to n can be employed. Taking into account the arbitrariness of all variations,

the discrete equations of motion can be obtained as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) \,, \tag{4.38a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n + \mathbf{P}^n = \mathrm{D}_1 L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) - \mathrm{D}_1 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) \,, \tag{4.38b}$$

$$-\mathbf{P}^n = \mathrm{D}_2 L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) - \mathrm{D}_2 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) \,, \tag{4.38c}$$

$$\mathbf{0} = \mathrm{D}_3 L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) - \mathrm{D}_3 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) \tag{4.38d}$$

for $n = 0, ..., N-1$ together with the discrete constraints

$$(\mathrm{D}_{\boldsymbol{\lambda}} L_\mathrm{d}^{\boldsymbol{\lambda}})(\mathbf{q}^n, \mathbf{q}^{n+1}) = \mathbf{0} \,, \tag{4.38e}$$

$$(\mathrm{D}_{\boldsymbol{\gamma}} \mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}})(\mathbf{q}^n, \mathbf{q}^{n+1})^\mathrm{T} \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) = \mathbf{0} \,, \tag{4.38f}$$

for $n = 0, ..., N-1$, where we made the assumption that velocities do not occur combined with the Langrange multipliers. This formally restricts our choices of $L_\mathrm{d}^{\boldsymbol{\lambda}}$ and $\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}$. Equation (4.38d) serves as a discrete version of the fiber derivative (4.6c) and links velocity to momentum variables. In total, we have obtained a set of $(4\,\mathrm{d} + 2\,m)$ equations for the unknowns $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}, \mathbf{P}^n, \mathbf{v}^{n+1}, \boldsymbol{\lambda}^n, \boldsymbol{\gamma}^n)$, which can be solved with Newton's method.

4.3.2 Proof of Symplecticness

Before going into further detail and exploring the governing equations for certain choices of the discrete augmented Lagrangian $L_\mathrm{d}^{\boldsymbol{\lambda}}$ or the kinematic right hand side vector $\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}$, we want to show that integration schemes which stem from (4.34) are indeed symplectic. In order to do so, we will derive the differential one forms corresponding to the DEL equations as well as the differentials of the discrete constraints. The latter ones are given by

$$\mathrm{D}_1(\mathrm{D}_{\boldsymbol{\lambda}} L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\mathbf{q}^n + \mathrm{D}_2(\mathrm{D}_{\boldsymbol{\lambda}} L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\mathbf{q}^{n+1} = \mathbf{0} \tag{4.39}$$

and

$$(\mathrm{D}_{\boldsymbol{\gamma}} \mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}})^\mathrm{T} \left(\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^n\right) + \left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) \cdot \left(\mathrm{D}_1(\mathrm{D}_{\boldsymbol{\gamma}} \mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}})\,\mathrm{d}\mathbf{q}^n + \mathrm{D}_2(\mathrm{D}_{\boldsymbol{\gamma}} \mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}})\,\mathrm{d}\mathbf{q}^{n+1}\right) = \mathbf{0} \,. \tag{4.40}$$

By computing appropriate wedge products several terms can be canceled out after some algebra. For the detailled procedure we refer to Appendix B.

We eventually obtain the relation

$$\begin{aligned}\mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n - \mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} = \\ + \mathrm{d}\boldsymbol{\lambda}^n \wedge \left(\mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_1 L_\mathrm{d}^{\boldsymbol{\lambda}})^\mathrm{T}\,\mathrm{d}\mathbf{q}^n + \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_2 L_\mathrm{d}^{\boldsymbol{\lambda}})^\mathrm{T}\,\mathrm{d}\mathbf{q}^{n+1}\right) \\ - \mathrm{d}\boldsymbol{\gamma}^n \wedge \Big(\mathrm{D}_{\boldsymbol{\gamma}}\mathbf{f}_\mathrm{d}^{\gamma\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^n) + \mathrm{D}_{\boldsymbol{\gamma}}(\mathrm{D}_1\mathbf{f}_\mathrm{d}^{\gamma})^\mathrm{T}(\mathbf{p}^{n+1} + \mathbf{P}^n)\,\mathrm{d}\mathbf{q}^n \\ + \mathrm{D}_{\boldsymbol{\gamma}}(\mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma})^\mathrm{T}(\mathbf{p}^{n+1} + \mathbf{P}^n)\,\mathrm{d}\mathbf{q}^{n+1}\Big)\ . \end{aligned} \tag{4.41}$$

It can be verified that the terms in brackets in (4.41) vanish due to the total differentials of the primary constraint (4.39) and of the secondary constraint (4.40), respectively. By simply interchanging the partial differentiations and applying the transposition of the Hessian matrices in (4.39) and (4.40), we obtain the symplecticness condition (2.104)

$$\mathrm{d}\mathbf{q}^{n+1} \wedge \mathrm{d}\mathbf{p}^{n+1} = \mathrm{d}\mathbf{q}^n \wedge \mathrm{d}\mathbf{p}^n\ . \tag{4.42}$$

Thus, the symplectic two-form $\Omega = \mathrm{d}\mathbf{q} \wedge \mathrm{d}\mathbf{p}$ is conserved along solutions of all integrators derived from the discrete action integral (4.34).

4.3.3 General Governing Equations

We now provide further details of the discrete augmented Lagrangian $L_\mathrm{d}^{\boldsymbol{\lambda}}$ introduced above. Specifically, one finds

$$L_\mathrm{d}^{\boldsymbol{\lambda}}(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = L_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) - \boldsymbol{\lambda}^n \cdot \mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1})\ , \tag{4.43}$$

where L_d denotes a discrete approximaton of the Lagrangian and $\mathbf{g}_\mathrm{d}$ denotes an arbitrary evaluation of the constraint on configuration level $\mathbf{g}(\mathbf{q})$. We can now derive the integration scheme emanating from (4.38a) to (4.38f) and, in order to do so, we eliminate the auxiliary momenta by rewriting (4.38c). We obtain

$$\mathbf{P}^n = \left(\mathbf{I} - \mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma\mathrm{T}}\right)^{-1}\left(\mathrm{D}_2 L_\mathrm{d}^{\boldsymbol{\lambda}} + \mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma\mathrm{T}}\mathbf{p}^{n+1}\right)\ , \tag{4.44}$$

where $\mathbf{I} \in \mathbb{R}^{d\times d}$ denotes the identity matrix. Calculating the discrete fiber derivative (4.38d) for the given discrete augmented Lagrangian (4.43), the velocities can be deduced as a function of the auxiliary momenta

$$\mathrm{D}_3 L_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = h\,\mathbf{M}\mathbf{v}^{n+1} = \mathrm{D}_3\mathbf{f}_\mathrm{d}^{\gamma}(\mathbf{q}^n, \mathbf{Q}^n, \mathbf{v}^{n+1})^\mathrm{T}\left(\mathbf{p}^{n+1} + \mathbf{P}^n\right)\ , \tag{4.45}$$

where we have assumed a standard Lagrangian in the form of (2.8) and $\mathbf{P}^n$ is defined by (4.44). Adding up (4.38b) and (4.38c) yields

$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_\mathrm{d}^{\boldsymbol{\lambda}} + \mathrm{D}_2 L_\mathrm{d}^{\boldsymbol{\lambda}} - (\mathrm{D}_1\mathbf{f}_\mathrm{d}^{\gamma} + \mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma})^\mathrm{T}\left(\mathbf{p}^{n+1} + \mathbf{P}^n\right)\ . \tag{4.46}$$

We eventually arrive at the discrete versions of the DAEs (4.6) as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \mathbf{f}_\mathrm{d}^\gamma \ , \tag{4.47a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_\mathrm{d}^\lambda + \mathrm{D}_2 L_\mathrm{d}^\lambda - h \ (\mathrm{D}_1 \mathbf{f}_\mathrm{d}^\gamma + \mathrm{D}_2 \mathbf{f}_\mathrm{d}^\gamma)^\mathrm{T} \mathbf{M} \mathbf{v}^{n+1} \ , \tag{4.47b}$$

$$h \, \mathbf{M} \mathbf{v}^{n+1} = \mathrm{D}_3 \mathbf{f}_\mathrm{d}^{\gamma\mathrm{T}} \left(\mathbf{p}^{n+1} + \left(\mathbf{I} - \mathrm{D}_2 \mathbf{f}_\mathrm{d}^{\gamma\mathrm{T}} \right)^{-1} \left(\mathrm{D}_2 L_\mathrm{d}^\lambda + \mathrm{D}_2 \mathbf{f}_\mathrm{d}^{\gamma\mathrm{T}} \mathbf{p}^{n+1} \right) \right) \ , \tag{4.47c}$$

$$\mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}) = \mathbf{0} \ , \tag{4.47d}$$

$$(\mathrm{D}_\gamma \mathbf{f}_\mathrm{d}^\gamma)^\mathrm{T} \mathbf{M} \mathbf{v}^{n+1} = \mathbf{0} \ , \tag{4.47e}$$

for stepping in time from $(\mathbf{q}^n, \mathbf{p}^n)$ to $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1})$ starting with initial conditions $\mathbf{q}^0$ and $\mathbf{p}^0$. In doing so, for every time step the suitable multipliers $\boldsymbol{\lambda}^n$ and $\boldsymbol{\gamma}^n$ are computed and (4.47c) serves as a discrete Legendre transform to calculate the unknown velocity $\mathbf{v}^{n+1}$. Note that one still has to specify L_d^λ and $\mathbf{f}_\mathrm{d}^\gamma$.

4.3.4 One-stage Theta Methods

A whole variety of choices for L_d^λ and $\mathbf{f}_\mathrm{d}^\gamma$ can be imagined. In this chapter we want to introduce two different options. Both are based on the general ansatz to evaluate the configuration at an intermediate point in time

$$\mathbf{q}^{n+\theta} = (1-\theta) \, \mathbf{q}^n + \theta \, \mathbf{q}^{n+1} \ . \tag{4.48}$$

The discrete augmented Lagrangian therefore takes the form

$$L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - \boldsymbol{\lambda}^n \cdot \mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}) \tag{4.49}$$

and the kinematic equation is chosen as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = h \, \mathbf{f}^\gamma(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) = h \, \mathbf{v}^{n+1} + h \, \mathbf{M}^{-1} \mathbf{G}(\mathbf{q}^{n+\theta})^\mathrm{T} \boldsymbol{\gamma}^n \ . \tag{4.50}$$

Having specified L_d^λ and $\mathbf{f}_\mathrm{d}^\gamma$, the partial derivatives can be written as

$$\mathrm{D}_1 L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = (1-\theta) \, \mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - D_1 \mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1})^\mathrm{T} \boldsymbol{\lambda}^n \ , \tag{4.51a}$$

$$\mathrm{D}_2 L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = \theta \, \mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - D_2 \mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1})^\mathrm{T} \boldsymbol{\lambda}^n \ , \tag{4.51b}$$

$$\mathrm{D}_3 L_\mathrm{d}^\lambda(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = \mathrm{D}_2 L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) = h \, \mathbf{M}^{-1} \mathbf{v}^{n+1} \ , \tag{4.51c}$$

$$\mathrm{D}_1 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = h \, (1-\theta) \, \mathrm{D}_1 \mathbf{f}^\gamma(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) \ , \tag{4.51d}$$

$$\mathrm{D}_2 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = h \, \theta \, \mathrm{D}_2 \mathbf{f}^\gamma(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) \ , \tag{4.51e}$$

$$\mathrm{D}_3 \mathbf{f}_\mathrm{d}^\gamma(\mathbf{q}^n, \mathbf{q}^{n+1}, \mathbf{v}^{n+1}) = h \, \mathbf{I} \ . \tag{4.51f}$$

Thus, together with (4.51f) the discrete fiber derivative (4.45) becomes

$$\mathbf{M} \mathbf{v}^{n+1} = \mathbf{p}^{n+1} + \mathbf{P}^n \tag{4.52}$$

and the discrete stationarity condition for the auxiliary momenta given in (4.38c) can be reformulated such that

$$\mathbf{P}^n = -\theta\, \mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) + D_2\mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1})^\mathrm{T}\boldsymbol{\lambda}^n + h\,\theta \mathrm{D}_1\mathbf{f}^\gamma(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1})^\mathrm{T}\left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) . \tag{4.53}$$

Evaluating the momentum equation (4.46) yields

$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - \left(\mathrm{D}_1\mathbf{g}_\mathrm{d} + \mathrm{D}_2\mathbf{g}_\mathrm{d}\right)^\mathrm{T}\boldsymbol{\lambda}^n - h\,\mathrm{D}_1\mathbf{f}^\gamma(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1})^\mathrm{T}\left(\mathbf{p}^{n+1} + \mathbf{P}^n\right) \tag{4.54}$$

and the auxiliary momenta can be deduced as

$$\mathbf{P}^n = -\theta\left(\mathbf{p}^{n+1} - \mathbf{p}^n\right) - \left(\theta\,\mathrm{D}_1\mathbf{g}_\mathrm{d}^\mathrm{T} - (1-\theta)\,\mathrm{D}_2\mathbf{g}_\mathrm{d}^\mathrm{T}\right)\boldsymbol{\lambda}^n . \tag{4.55}$$

Eventually, one can rewrite the right hand side of (4.52) as

$$\begin{aligned}\mathbf{p}^{n+1} + \mathbf{P}^n &= \theta\,\mathbf{p}^n + (1-\theta)\,\mathbf{p}^{n+1} - \left(\theta\,\mathrm{D}_1\mathbf{g}_\mathrm{d}^\mathrm{T} - (1-\theta)\,\mathrm{D}_2\mathbf{g}_\mathrm{d}^\mathrm{T}\right)\boldsymbol{\lambda}^n \\ &= \mathbf{p}^{n+1-\theta} - \left(\theta\,\mathrm{D}_1\mathbf{g}_\mathrm{d}^\mathrm{T} - (1-\theta)\,\mathrm{D}_2\mathbf{g}_\mathrm{d}^\mathrm{T}\right)\boldsymbol{\lambda}^n .\end{aligned} \tag{4.56}$$

In the last equation we could introduce the momenta evaluated at $t^{n+1-\theta}$, viz.

$$\mathbf{p}^{n+1-\theta} = \theta\,\mathbf{p}^n + (1-\theta)\,\mathbf{p}^{n+1} . \tag{4.57}$$

Moreover, there occur some additional terms which vanish under certain assumptions, for example if $\theta\,\mathrm{D}_1\mathbf{g}_\mathrm{d} = (1-\theta)\,\mathrm{D}_2\mathbf{g}_\mathrm{d}$. We will come back to this later when discussing detailed discretizations of the constraint equation. The above mentioned specifications enable us to write the DEL as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\,\mathbf{v}^{n+1} + h\,\mathbf{M}^{-1}\mathbf{G}(\mathbf{q}^{n+\theta})^\mathrm{T}\boldsymbol{\gamma}^n , \tag{4.58a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_\mathrm{d}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - \left(\mathrm{D}_1\mathbf{g}_\mathrm{d} + \mathrm{D}_2\mathbf{g}_\mathrm{d}\right)^\mathrm{T}\boldsymbol{\lambda}^n - h\sum_{k=1}^{m}\gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^{n+\theta})\mathbf{v}^{n+1} , \tag{4.58b}$$

$$\mathbf{M}\mathbf{v}^{n+1} = \mathbf{p}^{n+1-\theta} - \left(\theta\,\mathrm{D}_1\mathbf{g}_\mathrm{d}^\mathrm{T} - (1-\theta)\,\mathrm{D}_2\mathbf{g}_\mathrm{d}^\mathrm{T}\right)\boldsymbol{\lambda}^n , \tag{4.58c}$$

$$\mathbf{g}_\mathrm{d}(\mathbf{q}^n, \mathbf{q}^{n+1}) = \mathbf{0} , \tag{4.58d}$$

$$\mathbf{G}(\mathbf{q}^{n+\theta})\mathbf{v}^{n+1} = \mathbf{0} . \tag{4.58e}$$

In the following we want to distinguish two different options for the evaluation of the constraints on configuration level.

Option A: Intermediate Constraint Evaluation

This option simply computes the constraint function in the same intermediate configuration, where we have also evaluated the other quantities. Thus,

$$\mathbf{g}_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = h\, \mathbf{g}(\mathbf{q}^{n+\theta}) \tag{4.59}$$

and the spatial derivatives yield

$$\mathrm{D}_1\mathbf{g}_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = h\,(1-\theta)\,\mathbf{G}(\mathbf{q}^{n+\theta})\ , \tag{4.60a}$$
$$\mathrm{D}_2\mathbf{g}_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = h\,\theta\,\mathbf{G}(\mathbf{q}^{n+\theta})\ . \tag{4.60b}$$

Hence, the additional term in (4.56) cancels out and we obtain

$$\mathbf{p}^{n+1} + \mathbf{P}^n = \mathbf{p}^{n+1-\theta} = \mathbf{M}\mathbf{v}^{n+1} \tag{4.61}$$

for the discrete Legendre transformation. Summing up both partial derivatives leads to vanishing terms with θ such that we can simplify the momentum update equation. The resulting discrete equations of motion read

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\,\mathbf{v}^{n+1} + h\,\mathbf{M}^{-1}\mathbf{G}(\mathbf{q}^{n+\theta})^{\mathrm{T}}\boldsymbol{\gamma}^n\ , \tag{4.62a}$$
$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_{\mathrm{d}}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - h\,\mathbf{G}(\mathbf{q}^{n+\theta})^{\mathrm{T}}\boldsymbol{\lambda}^n - h\sum_{k=1}^{m}\gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^{n+\theta})\mathbf{v}^{n+1}\ , \tag{4.62b}$$
$$\mathbf{M}\mathbf{v}^{n+1} = \mathbf{p}^{n+1-\theta}\ , \tag{4.62c}$$
$$\mathbf{g}(\mathbf{q}^{n+\theta}) = \mathbf{0}\ , \tag{4.62d}$$
$$\mathbf{G}(\mathbf{q}^{n+\theta})\mathbf{v}^{n+1} = \mathbf{0}\ . \tag{4.62e}$$

One severe drawback of this method is that for $\theta \neq \{0, 1\}$ the constraint on configuration level is enforced at intermediate times such that the constraint is not fulfilled numerically in the discrete points in time. For example $\theta = 0.5$ leads to an integration scheme, which can be interpreted as the application of the midpoint-rule to the EL equations of the GGL functional (cf. (4.6)). For the detailled DEL and a numerical investigation see Appendix C.1.

However, $\theta = 0$ is not an admissible value as (4.62d) would be redundant and the set of equations would become singular. Moreover, $\theta = 1$ is neither admissible since the constraint on momentum level in this case becomes

$$\mathbf{G}(\mathbf{q}^{n+1})\mathbf{M}^{-1}\mathbf{p}^n = \mathbf{0}\ , \tag{4.63}$$

which is hard to fulfill. For $n = 0$ the constraint forces which are proportional to $\mathbf{G}(\mathbf{q}^{n+1})$ have to be perpendicular to the initial momentum $\mathbf{p}^0$, which is usually chosen such that it is perpendicular to the initial constraint forces. In general, this leads to a singular set of equations. Alleviating this issue by simply replacing (4.62d) and (4.62e) by endpoint evaluations leads to a *modified theta-integrator* which is neither symplectic

nor a variational integrator. For a numerical investigation and the detailed DEL refer to Appendix C.2. Let us now proceed with another choice for the discrete constraint.

Option B: Trapezoidal Constraint Evaluation

For this option, another parameter ϑ is introduced to control the evaluation of the constraint on configuration level as

$$\mathbf{g}_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = h \left((1-\vartheta)\, \mathbf{g}(\mathbf{q}^n) + \vartheta\, \mathbf{g}(\mathbf{q}^{n+1}) \right) . \tag{4.64}$$

Note that $\vartheta = 0$ is not an admissible choice, since the constraint would only be enforced for already known state $\mathbf{q}^n$. The discrete constraint equation (4.38e) would make the system of equations become singular again. The derivatives of the discrete constraint (4.64) read

$$\mathrm{D}_1 \mathbf{g}_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = h\,(1-\vartheta)\, \mathbf{G}(\mathbf{q}^n) , \tag{4.65a}$$
$$\mathrm{D}_2 \mathbf{g}_{\mathrm{d}}(\mathbf{q}^n, \mathbf{q}^{n+1}) = h\,\vartheta\, \mathbf{G}(\mathbf{q}^{n+1}) . \tag{4.65b}$$

We can assume that the initial condition $\mathbf{q}_0 = \mathbf{q}(t=0)$ fulfills the constraint exactly and that $\vartheta = 0$ is not admissible. Thus, the discrete constraint equation in this method enforces only the configuration at t^{n+1}. Hence, the discrete equations of motion become

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\, \mathbf{v}^{n+1} + h\, \mathbf{M}^{-1} \mathbf{G}(\mathbf{q}^{n+\theta})^{\mathrm{T}} \boldsymbol{\gamma}^n , \tag{4.66a}$$
$$\begin{aligned} \mathbf{p}^{n+1} - \mathbf{p}^n = {} & \mathrm{D}_1 L_{\mathrm{d}}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - h \left((1-\vartheta)\, \mathbf{G}(\mathbf{q}^n) + \vartheta\, \mathbf{G}(\mathbf{q}^{n+1}) \right)^{\mathrm{T}} \boldsymbol{\lambda}^n \\ & - h \sum_{k=1}^{m} \gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^{n+\theta}) \mathbf{v}^{n+1} , \end{aligned} \tag{4.66b}$$
$$\mathbf{M}\mathbf{v}^{n+1} = \mathbf{p}^{n+1-\theta} - h \left(\theta\,(1-\vartheta)\, \mathbf{G}(\mathbf{q}^n)^{\mathrm{T}} - (1-\theta)\,\vartheta\, \mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}} \right) \boldsymbol{\lambda}^n , \tag{4.66c}$$
$$\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{0} , \tag{4.66d}$$
$$\mathbf{G}(\mathbf{q}^{n+\theta}) \mathbf{v}^{n+1} = \mathbf{0} . \tag{4.66e}$$

Therefore, the discrete momenta and velocities are not aligned since the additional term in the discrete Legendre transformation does not vanish. This avoids the numerical drawbacks of option A, which made an evaluation of the constraints at t^{n+1} impossible. Consequently, we can choose $\theta = 1$ in order to capture the constraint on velocity level and on configuration level while maintaining the symplectic nature of the integration scheme. Furthermore $\vartheta = 0.5$ has been shown to provide good performances. For this

specific choice of the parameters the discrete EL equations read

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\,\mathbf{v}^{n+1} + h\,\mathbf{M}^{-1}\mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}}\boldsymbol{\gamma}^n \;, \tag{4.67a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_{\mathrm{d}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) - \frac{h}{2}\left(\mathbf{G}(\mathbf{q}^n) + \mathbf{G}(\mathbf{q}^{n+1})\right)^{\mathrm{T}}\boldsymbol{\lambda}^n - h\sum_{k=1}^{m}\gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^{n+1})\mathbf{v}^{n+1} \;, \tag{4.67b}$$

$$\mathbf{M}\mathbf{v}^{n+1} = \mathbf{p}^n - \frac{h}{2}\mathbf{G}(\mathbf{q}^n)^{\mathrm{T}}\boldsymbol{\lambda}^n \;, \tag{4.67c}$$

$$\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{0} \;, \tag{4.67d}$$

$$\mathbf{G}(\mathbf{q}^{n+1})\mathbf{v}^{n+1} = \mathbf{0} \;. \tag{4.67e}$$

for $n = 0, ..., N-1$. Another possible choice of parameters would be $\theta = \vartheta = 0.5$ which causes both constraints to be violated in discrete time steps but reduces the symplectic energy oscillations. More on that specific integrator can be found in Appendix C.1.

4.3.5 Numerical Example: Steady Precession of a Gyroscopic Top

The objective of this subsection is to analyze the behavior of the previously derived symplectic one-stage theta method with a trapezoidal constraint evaluation (option B) by means of a numerical example. The perfomances of option A and the corresponding modified integrator are presented in Appendix C.1 and Appendix C.2, respectively. In this example we investigate the motion of a rigid body according to the framework given in Section 3.4 where the rigidity is described by the orthonormality condition of three directors $\{\mathbf{d}_i\}$ positioned in the center of mass $\boldsymbol{\varphi}$ (cf. Fig. 3.1 and relation (3.53) for comparison). Specifically, a gyroscopic top, as depicted in Fig. 4.9, has been investigated for a total simulation time of $T = 2\,\mathrm{s}$ with a time step size of $h = 0.001\,\mathrm{s}$ computed with Option B of the symplectic one-stage theta method with $\theta = 1$ and $\vartheta = 0.5$.

The total mass of the top amounts to $m = 0.7069\,\mathrm{kg}$ and the momenta of inertia read $J_1 = J_2 = J_3 = 5.3014 \cdot 10^{-4}\,\mathrm{kg\,m^2}$ which corresponds to a cylinder with mass density $\rho = 2700\,;\mathrm{kg/m^3}$, height $a = 0.1\mathrm{m}$, top radius $r = a/2$ and a location of the center of mass along the symmetry axis $l = 3/4\,a$. In this case, the momenta of inertia can be computed via

$$J_1 = J_2 = \frac{3}{80}m(4r^2 + a^2) \;, \tag{4.68a}$$

$$J_3 = \frac{3}{10}mr^2 \;, \tag{4.68b}$$

and the total mass is given by

$$m = \frac{1}{3}\rho\pi r^2 a \;. \tag{4.69}$$

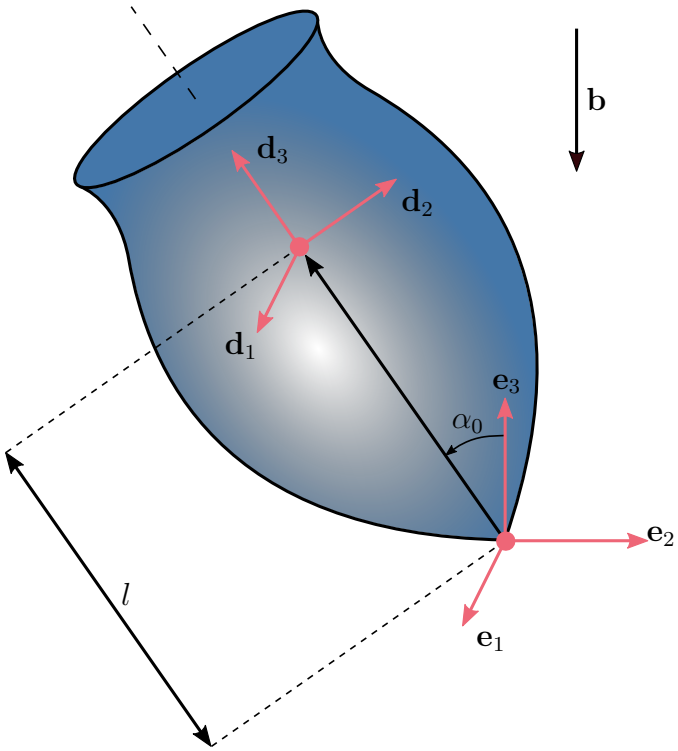

Figure 4.9: Initial configuration of the gyroscopic top

Gravitation acts in the negative $\mathbf{e}_3$-direction with

$$\mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ -9.81 \end{bmatrix} \mathrm{m/s^2} \tag{4.70}$$

such that the potential energy of the system only depends on the position of the center of mass $\boldsymbol{\varphi}$, viz.

$$V(\mathbf{q}) = \hat{V}(\boldsymbol{\varphi}) = m\,\mathbf{b} \cdot \boldsymbol{\varphi} \ . \tag{4.71}$$

It is crucially important that the top is subject to an additional constraint

$$g_{\mathrm{cm}}(\mathbf{q}) = \boldsymbol{\varphi} - l\mathbf{d}_3 = 0 \ , \tag{4.72}$$

which fixes the tip of the gyroscopic top to the origin of $\{\mathbf{e}_i\}$ by enforcing that the center of mass is located on the axis of symmetry with a distance of l to the origin. The initial nutation angle is $\alpha_0 = \pi/3$ and the gyroscopic top is subject to an initial angular velocity vector

$$\boldsymbol{\omega}_0 = \omega_{\mathrm{p}}\,\mathbf{e}_3 + \omega_{\mathrm{s}}\,\mathbf{d}_3 \ , \tag{4.73}$$

where the initial precession rate is chosen as $\omega_p = 10\,\mathrm{s}^{-1}$ and the initial spin rate for the

case of a steady precession can be computed via the relation

$$\omega_\mathrm{s} = \frac{m\,g\,l}{J_3\,\omega_\mathrm{p}} + \frac{J_1 + m\,l^2 - J_3}{J_3}\,\omega_p\,\cos(\alpha_0) \tag{4.74}$$

(cf. p. 221 in Goldstein [2]), which in this case amounts to $\omega_\mathrm{s} = 135.6\,\mathrm{s}^{-1}$. Note that $g = 9.81\,\mathrm{m/s^2}$ denotes the magnitude of gravitational acceleration here. The transformation from the global $\mathbf{e}_i$ coordinate system to the initially inclined system can easily be done by the use of a rotation matrix $\mathbf{R}_0 \in SO(3)$ with the well-known property $\mathbf{R}_0^\mathrm{T} = \mathbf{R}_0^{-1}$. For the present case this reads

$$\mathbf{R}_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha_0) & -\sin(\alpha_0) \\ 0 & \sin(\alpha_0) & \cos(\alpha_0) \end{bmatrix}\,, \tag{4.75}$$

which prescribes a rotation about the $\mathbf{e}_1$-axis with the angle α_0 as can be seen in Fig. 4.9. Thus, the initial velocities of the center of mass and the directors can be computed by taking the cross product with the initial configuration

$$\dot{\boldsymbol{\varphi}}(t=0) = \boldsymbol{\omega}_0 \times \boldsymbol{\varphi}(t=0)\,, \tag{4.76a}$$

$$\dot{\mathbf{d}}_\mathrm{i}(t=0) = \boldsymbol{\omega}_0 \times \mathbf{d}_\mathrm{i}(t=0)\,, \tag{4.76b}$$

where $\boldsymbol{\omega}_0$ can be transformed to the global coordinate system first with the aid of $\mathbf{R}_0$ to simplify the computation. The Newton's method's tolerance has been set to $\varepsilon_\mathrm{tol} = 10^{-9}$. The computation has been performed using the *metis* code, which is available at [58]. By ensuring the condition for a steady precession (4.74) the center of mass is rotating on

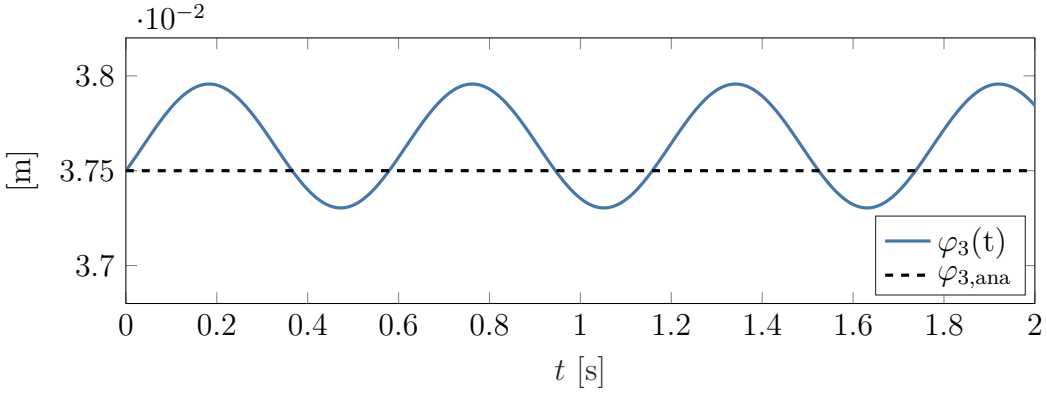

Figure 4.10: Vertical coordinate of center of mass

a constant height φ_3 around the vertical axis since gravitational forces and restabilizing effects due to the rotation are in an equilibrium. The horizontal coordinate of the center of mass φ_3 can thus be regarded as an analytical reference to the solutions. The results given by the symplectic integration scheme oscillates around this analytical solution, as can be seen in Fig. 4.10. The total energy of the system is not conserved along the solutions of this integration scheme (cf. Fig. 4.12). However, as it is typical for symplectic methods (cf. Fig. 16 in Lew et al. [18]), $H(t)$ oscillates around its true value from one

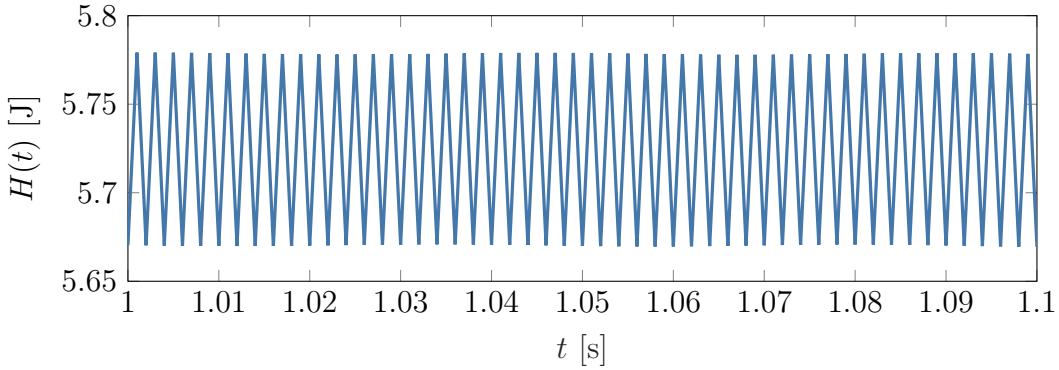

Figure 4.11: $H(t)$ for $t \in [1.0\,\mathrm{s}\ ,\ 1.1\,\mathrm{s}]$

time step to another and the energy error remains stable. This oscillation is shown for the time interval from $t = 1\,\mathrm{s}$ until $t = 1.1\,\mathrm{s}$ in Fig. 4.11. Moreover, Fig. 4.14 displays the increments in H from one time step to another, which remains bounded during the whole simulation. Furthermore, as the gyroscopic top is subject to external forces acting in the $\mathbf{e}_3$-direction, the symmetry of the system reduces to a conservation of the angular momentum about the $\mathbf{e}_3$-axis such that $L_3 = \text{constant}$. This is correctly captured by the symplectic method and can be seen in Fig. 4.13. Differences in L_3 from one point in time to another are close to computer precision (cf. Fig. 4.15). By design, the constraints

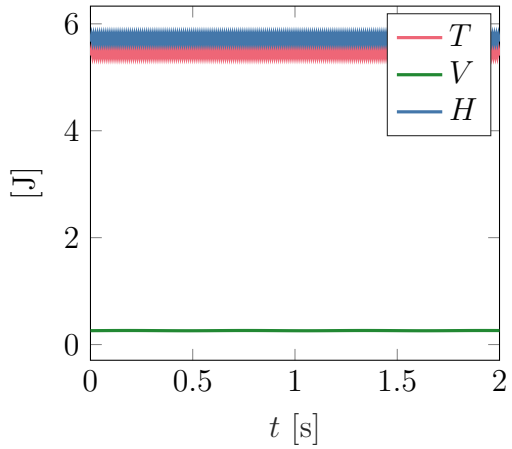

Figure 4.12: Energy quantities

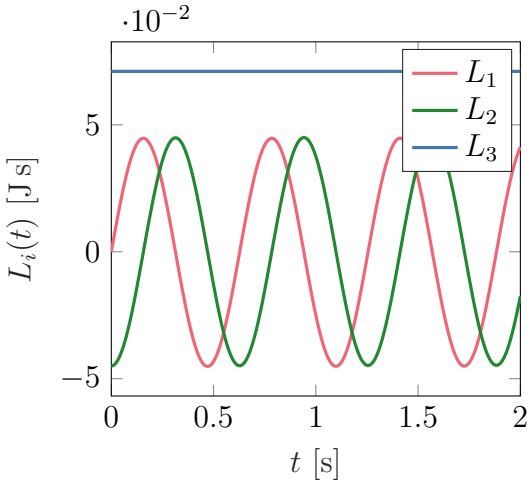

Figure 4.13: Angular momentum

both on configuration and on velocity level are identically fulfilled which can be observed in Fig. 4.16 and Fig. 4.17, respectively. Hence, the symplectic one-stage theta method with option B conserves the constraint phase space.

In an analogous manner to the previous example discussed in Sec. 4.2.3 we can now analyze the h-convergence of the one-stage theta methods for the current example. Therefore we have investigated the relative error in the vertical coordinate of the center of mass, which is supposed to remain constant, at time $t = 0.001\,\mathrm{s}$. In Fig. 4.18 we display the

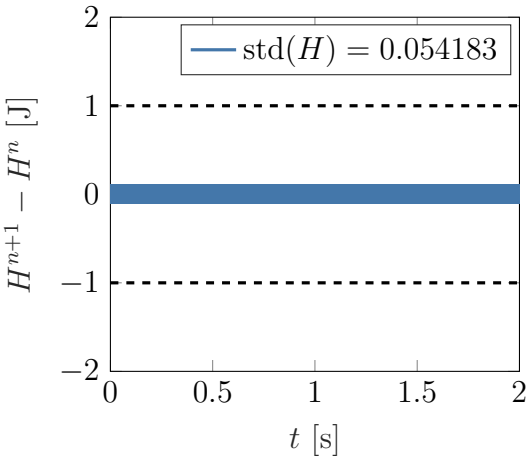

Figure 4.14: Hamiltonian difference

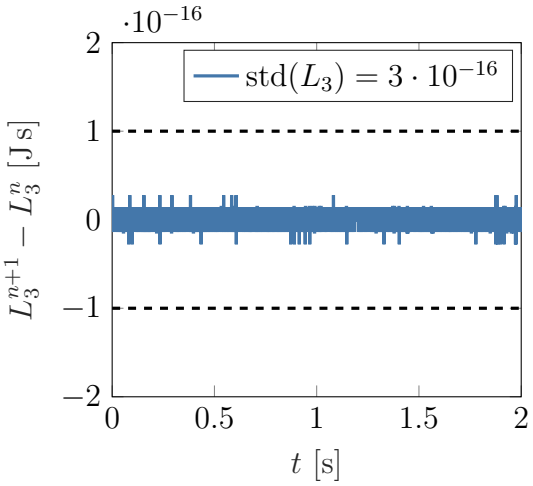

Figure 4.15: Angular momentum difference

relative error

$$e = \frac{|\varphi_3(t = 0.001\,\mathrm{s}) - \varphi_{3,\mathrm{ana}}|}{\varphi_{3,\mathrm{ana}}} \tag{4.77}$$

for the different integration schemes and different time step sizes h. It becomes visible that the one-stage theta method with a trapezoidal evaluation of the constraint ("Option A") is first order accurate and behaves similarly to the first variational integrator from Section 4.2 ("GGL-VI") and the constrained symplectic Euler B scheme ("CSE-B"), which has been introduced in Section 3.3.2. If we recall the one-stage theta method with an intermediate evaluation ("Option B") and set $\theta = 0.5$, this leads to a second order scheme with comparably small errors close to the tolerance value of Newton's method. For further details see Appendix C.1. Moreover, results for the modified theta integrator, which is not symplectic but satisfies both primary and secondary constraints, have been displayed as well. This method is second order accurate and yields the smallest errors. It can be deduced that with the present family of integrators it is not possible to achieve a second order accurate method while exactly capturing the systems' constraints. However, we want to emphasize that the introduced variational integration schemes are symplectic and inherit the conservation of the angular momentum of continuous dynamic systems.

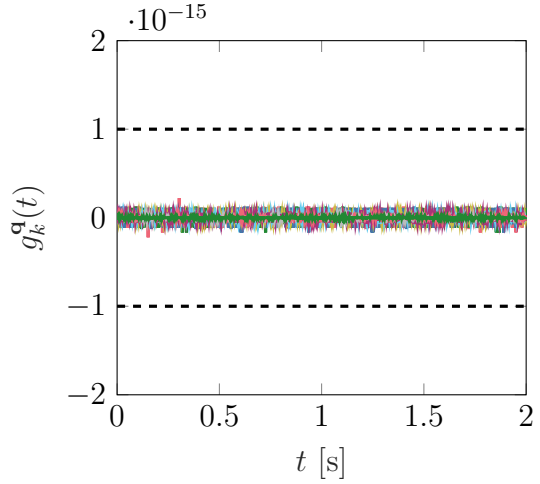

Figure 4.16: Constraints on configuration level

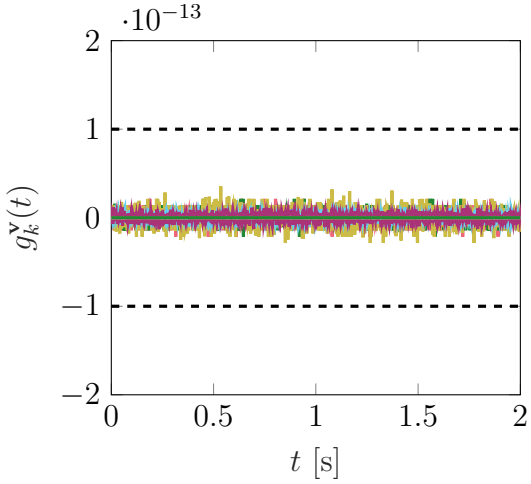

Figure 4.17: Constraints on velocity level

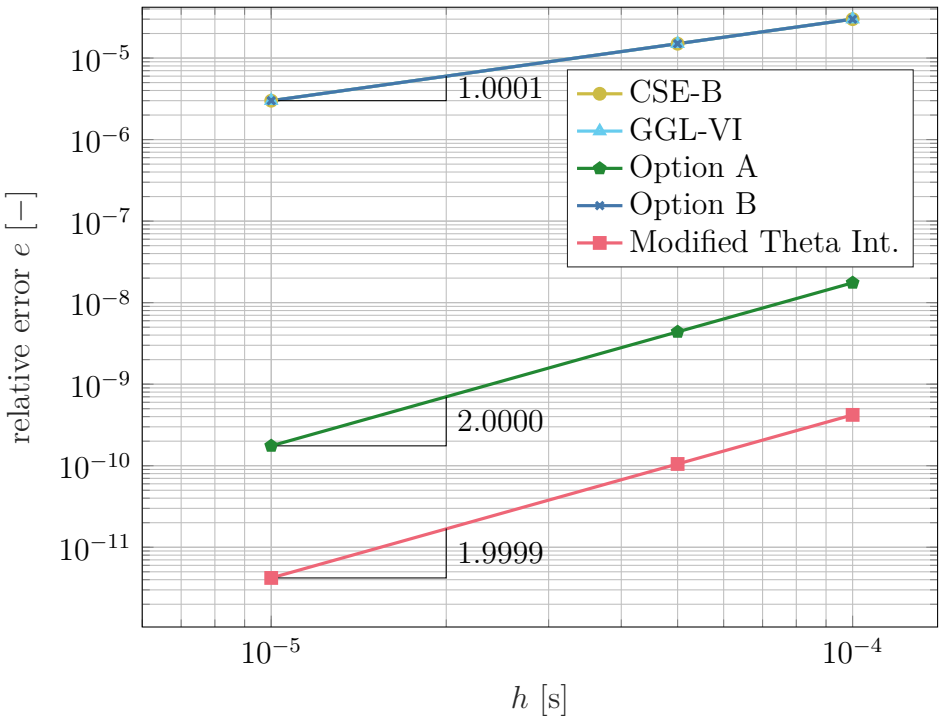

Figure 4.18: h-convergence of relative error in $\mathbf{q}$

4.4 Energy-Momentum Scheme

As the DAEs of the GGL functional (4.10) have Hamiltonian structure, we are able to derive an Energy-Momentum preserving integration scheme, which conserves the symmetries and the momentum maps of the underlying continuous system, i.e. both constraints as well as total energy and angular momentum. However, this method does not inherit the symplectic structure of Hamiltonian systems. The main idea is to directly discretize the EL equations by introducing the concept of *discrete gradients*. It was Gonzalez [33] who has derived energy-momentum-conserving integration schemes for the dynamics of unconstrained systems (cf. Gonzalez [33]) and later generalized his framework for constrained systems (cf. Gonzalez [14]).

We introduce the main idea of discrete derivatives in the first part (cf. Sec. 4.4.1) and later on derive an EM scheme for the equations of motion given by the newly proposed functional (cf. Sec. 4.4.2). In the next part, the underlying conservation properties will be shown (cf. Sec. 4.4.3). Towards the end of the current section, the motion of a dynamical system will be solved numerically with the presented EM integrator in Section 4.4.4.

4.4.1 General Concept of Discrete Derivatives

The following deductions mainly follow along the work by Gonzalez. All necessary proofs can be found there and are omitted here. The structure of discrete gradient emanates from the general idea of difference quotients (cf. Greenspan [30]) as

$$\mathrm{D}f(x^n) \approx \frac{f(x^{n+1}) - f(x^n)}{x^{n+1} - x^n} \ . \tag{4.78}$$

For functions $f : \mathcal{P} \to \mathbb{R}$ defined on a subset of the $2d$-dimensional Euclidean space, e.g. the phase space, Gonzalez [33] has introduced a definition for a discrete derivative. With $\mathbf{x}, \mathbf{y} \in \mathcal{P}$, the discrete derivative approximates the exact gradient (A.2) as

$$\mathsf{D}f(\mathbf{x}, \mathbf{y}) = \mathrm{D}f(\mathbf{z}) + \frac{f(\mathbf{y}) - f(\mathbf{x}) - \mathrm{D}f(\mathbf{z}) \cdot \mathbf{v}}{\| \mathbf{v} \|^2} \mathbf{v} \ , \tag{4.79}$$

where $\mathbf{z} = (\mathbf{x} + \mathbf{y})/2$ and $\mathbf{v} = \mathbf{y} - \mathbf{x}$ and $\| \bullet \|$ denotes the standard Euclidean norm. The general discrete derivative meets two crucial conditions:

1. *Directionality condition*

$$\mathsf{D}f(\mathbf{x}, \mathbf{y}) \cdot \mathbf{v} = f(\mathbf{y}) - f(\mathbf{x}) \tag{4.80}$$

   and

2. *Consistency condition*

$$\mathsf{D}f(\mathbf{x}, \mathbf{y}) = \mathrm{D}f(\mathbf{z}) + \mathcal{O}(\| \mathbf{v} \|) \ . \tag{4.81}$$

The directionality condition (4.80) can be motivated from the Greenspan formula (4.78) and from the orthogonality condition of gradients of first integrals of Hamiltonian systems (2.33). The consistency condition states that in the limit $\mathbf{x} \to \mathbf{y}$ the discrete derivative tends to the exact gradient evaluated in the midpoint $\mathbf{z}$ and the truncation error terms approach zero with at least first order. Thus, the discrete gradient is a second order accurate approximation to the analytic gradient. Consisteny is crucial for the construction of converging time integration schemes. Note that for the one-dimensional special case with $d = 1$ the discrete gradient simplifies to

$$\mathsf{D}f(x, y) = \frac{f(y) - f(x)}{y - x} \ , \tag{4.82}$$

which is in good agreement with the Greenspan formula (4.78). Now let us assume the function to be *G-invariant*

$$f(\mathbf{z}) = f(\mathbf{\Phi}_{\mathbf{g}}(\mathbf{z})) \qquad \forall \mathbf{g} \in \mathcal{G} \tag{4.83}$$

with $\Phi : \mathcal{G} \times \mathcal{P} \to \mathcal{P}$ being a regular symplectic action of $\mathcal{G}$ on $\mathcal{P}$ and $\mathbf{\Phi}_{\mathbf{g}}(\mathbf{z}) = \mathbf{\Phi}(\mathbf{g}, \mathbf{z})$. If $\pi_i : \mathcal{P} \to \mathbb{R}$ are invariants of $\mathcal{G}$ which are at most quadratic it is straightforward to accumulate them in a vector $\boldsymbol{\pi} = [\pi_1 \ \pi_2 \ ... \ \pi_m]^{\mathrm{T}}$. Under that assumption, we can reformulate f as a function of those invariants with $f(\mathbf{z}) = \tilde{f}(\boldsymbol{\pi}(\mathbf{z}))$. Accordingly, a discrete derivative for those functions can be written in the form

$$\mathsf{D}^{\mathrm{G}} f(\mathbf{x}, \mathbf{y}) = \mathrm{D}\boldsymbol{\pi}(\mathbf{z})^{\mathrm{T}} \, \mathsf{D}\tilde{f}(\boldsymbol{\pi}(\mathbf{x}), \boldsymbol{\pi}(\mathbf{y})) = \sum_{i=1}^{m} \mathrm{D}\pi_i(\mathbf{z}) \cdot \mathsf{D}\tilde{f}(\pi_i(\mathbf{x}), \pi_i(\mathbf{y})) \ , \tag{4.84}$$

where the superscript G indicates that one speaks of *G-equivariant* discrete derivatives. Additionally to the conditions above (cf. (4.80) and (4.81)), G-equivariant discrete derivatives underlie two more conditions:

3. *Equivariance condition*

$$\mathsf{D}f(\mathbf{\Phi}_{\mathbf{g}}(\mathbf{x}), \mathbf{\Phi}_{\mathbf{g}}(\mathbf{y})) = \mathrm{D}\mathbf{\Phi}_{\mathbf{g}}(\mathbf{z})^{\mathrm{T}} \mathsf{D}^{\mathrm{G}} f(\mathbf{x}, \mathbf{y}) \tag{4.85}$$

   and

4. *Orthogonality condition*

$$\mathsf{D}^{\mathrm{G}} f(\mathbf{x}, \mathbf{y}) \cdot \boldsymbol{\xi}_P(\mathbf{z}) = 0 \ , \tag{4.86}$$

where in the last equation $\boldsymbol{\xi}_P$ is the infinitesimal generator defined in (2.38). Both conditions, (4.85) and (4.86), are motivated by properties of standard derivatives of G-invariant functions.

4.4.2 EM Scheme for the GGL Functional

This section covers an EM conserving integration scheme that fulfills both the constraint on configuration level (4.6d) and the constraint on momentum level (4.6e). For at most quadratic constraints and potentials the method reduces to a midpoint evaluation of the differential equations of motion (4.6a) to (4.6c). A midpoint integration scheme of that kind has already been used by Betsch et al. [54] and later applied to the framework of geometrically exact beam formulations [61]

To generate a structure preserving integration scheme, we assume a Hamiltonian system with symmetries and that the constraints are G-invariant in order to apply the discrete derivative to the Hamiltonian equations of motion of the GGL functional (4.10) in the following fashion

$$\mathbf{z}^{n+1} - \mathbf{z}^n = h\,\mathsf{D}^{\mathrm{G}}\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{z}^n, \mathbf{z}^{n+1}) \;, \tag{4.87a}$$

$$\mathbf{g}^{\mathbf{q}}(\mathbf{q}^{n+1}) = \mathbf{0} \;, \tag{4.87b}$$

$$\mathbf{g}^{\mathbf{v}}(\mathbf{z}^{n+1}) = \mathbf{0} \;, \tag{4.87c}$$

where the G-equivariant discrete derivative can be computed via (4.84). By considering the augmented Hamiltonian corresponding to the GGL-functional given in (4.8), this can be specified as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\mathsf{D}^{\mathrm{G}}_{\mathbf{p}} H(\mathbf{z}^n, \mathbf{z}^{n+1}) + h\sum_{k=1}^{m} \gamma_k^{n+1} \mathsf{D}^{\mathrm{G}}_{\mathbf{p}} g_k^{\mathbf{v}}(\mathbf{z}^n, \mathbf{z}^{n+1}) \;, \tag{4.88a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = -h\mathsf{D}^{\mathrm{G}}_{\mathbf{q}} H(\mathbf{z}^n, \mathbf{z}^{n+1}) - h\sum_{k=1}^{m} \lambda_k^{n+1} \mathsf{D}^{\mathrm{G}} g_{\mathbf{q}}(\mathbf{q}^n, \mathbf{q}^{n+1}) - h\sum_{k=1}^{m} \gamma_k^{n+1} \mathsf{D}^{\mathrm{G}}_{\mathbf{q}} g_k^{\mathbf{v}}(\mathbf{z}^n, \mathbf{z}^{n+1}) \;, \tag{4.88b}$$

$$\mathbf{g}^{\mathbf{q}}(\mathbf{q}^{n+1}) = \mathbf{0} \;, \tag{4.88c}$$

$$\mathbf{g}^{\mathbf{v}}(\mathbf{z}^{n+1}) = \mathbf{0} \;, \tag{4.88d}$$

for $n = 0, ..., N-1$. These equations represent $2(d+m)$ relations for the unknowns $(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}, \boldsymbol{\lambda}^{n+1}, \boldsymbol{\gamma}^{n+1})$ in every time step, which can be solved with Newton's method. In order to apply G-equivariant discrete derivatives we must rewrite the augmented Hamiltonian in terms of the invariants of $\mathbf{z}$ under the action of $\mathcal{G}$ such that $\mathcal{H}_{\boldsymbol{\lambda\gamma}}(\mathbf{q}, \mathbf{p}) = \tilde{\mathcal{H}}_{\boldsymbol{\lambda\gamma}}(\boldsymbol{\pi}(\mathbf{q}, \mathbf{p}))$. For the mathematical pendulum that we have already analyzed in Section 4.2.3 this exemplarily yields

$$\tilde{\mathcal{H}}_{\boldsymbol{\lambda\gamma}}(\pi_i(\mathbf{q}, \mathbf{p})) = T(\pi_3) + V(\pi_1) + \boldsymbol{\lambda} \cdot \mathbf{g}^{\mathbf{q}}(\pi_1) + \boldsymbol{\gamma} \cdot \mathbf{g}^{\mathbf{v}}(\pi_2) \tag{4.89}$$

with the three invariants being

$$\pi_1(\mathbf{q}) = \mathbf{q} \cdot \mathbf{q} \;, \tag{4.90a}$$

$$\pi_2(\mathbf{q}, \mathbf{p}) = \mathbf{q} \cdot \mathbf{p} \;, \tag{4.90b}$$

$$\pi_3(\mathbf{p}) = \mathbf{p} \cdot \mathbf{p} \;. \tag{4.90c}$$

Thus, for this special case of the mathematical pendulum, the equations of motion can

be simplified in view of (4.89) as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\,\mathbf{M}^{-1}\mathbf{p}^{\mathrm{n}+1/2} + h\sum_{k=1}^{m}\gamma_k^{n+1}\mathsf{D}g_k^{\mathbf{v}}(\pi_2^{n+1},\pi_2^n)\,\mathbf{q}^{n+1/2} \quad , \tag{4.91a}$$

$$\begin{aligned}\mathbf{p}^{n+1} - \mathbf{p}^n = &-2h\,\mathsf{D}V(\pi_1^{n+1},\pi_1^n)\,\mathbf{q}^{n+1/2} \\ &- h\sum_{k=1}^{m}\left(\lambda_k^{n+1}\mathsf{D}g_k^{\mathbf{q}}(\pi_1^{n+1},\pi_1^n)\,\mathbf{q}^{n+1/2} + \gamma_k^{n+1}\mathsf{D}g_k^{\mathbf{v}}(\pi_2^{n+1},\pi_2^n)\,\mathbf{p}^{n+1/2}\right) \quad ,\end{aligned} \tag{4.91b}$$

$$\mathbf{g}^{\mathbf{q}}(\pi_1^{n+1}) = \mathbf{0} \ , \tag{4.91c}$$

$$\mathbf{g}^{\mathbf{v}}(\pi_2^{n+1}) = \mathbf{0} \ . \tag{4.91d}$$

The integration scheme above conserves phase space (both constraints vanish identically), the system's Hamiltonian H and its angular momentum $\mathbf{L}$ in every time-step.

4.4.3 Conservation Properties

To prove the discrete conservation of the total energy in terms of the Hamiltonian (2.106), we take the scalar product of (4.88a) with $\mathbf{p}^{n+1} - \mathbf{p}^n$ and subtract the inner product of (4.88b) with $\mathbf{q}^{n+1} - \mathbf{q}^n$:

$$\begin{aligned}0 =&h\,\mathsf{D}_{\mathbf{p}}^{\mathrm{G}}H(\mathbf{z}^n,\mathbf{z}^{n+1})\cdot(\mathbf{p}^{n+1}-\mathbf{p}^n) + h\,\mathsf{D}_{\mathbf{q}}^{\mathrm{G}}H(\mathbf{z}^n,\mathbf{z}^{n+1})\cdot(\mathbf{q}^{n+1}-\mathbf{q}^n) \\ &+ h\sum_{k=1}^{m}\lambda_k^{n+1}\mathsf{D}^{\mathrm{G}}g_{\mathbf{q}}(\mathbf{q}^n,\mathbf{q}^{n+1})\cdot(\mathbf{q}^{n+1}-\mathbf{q}^n) \\ &+ h\sum_{k=1}^{m}\gamma_k^{n+1}\mathsf{D}_{\mathbf{p}}^{\mathrm{G}}g_k^{\mathbf{v}}(\mathbf{z}^n,\mathbf{z}^{n+1})\cdot(\mathbf{p}^{n+1}-\mathbf{p}^n) + h\sum_{k=1}^{m}\gamma_k^{n+1}\mathsf{D}_{\mathbf{q}}^{\mathrm{G}}g_k^{\mathbf{v}}(\mathbf{z}^n,\mathbf{z}^{n+1})\cdot(\mathbf{q}^{n+1}-\mathbf{q}^n) \ ,\end{aligned} \tag{4.92}$$

where it is possible to combine derivatives with respect to both positions and momenta as

$$\begin{aligned}0 =&h\,\mathsf{D}^{\mathrm{G}}H(\mathbf{z}^n,\mathbf{z}^{n+1})\cdot(\mathbf{z}^{n+1}-\mathbf{z}^n) + h\sum_{k=1}^{m}\lambda_k^{n+1}\mathsf{D}^{\mathrm{G}}g_{\mathbf{q}}(\mathbf{q}^n,\mathbf{q}^{n+1})\cdot(\mathbf{q}^{n+1}-\mathbf{q}^n) \\ &+ h\sum_{k=1}^{m}\gamma_k^{n+1}\mathsf{D}^{\mathrm{G}}g_k^{\mathbf{v}}(\mathbf{z}^n,\mathbf{z}^{n+1})\cdot(\mathbf{z}^{n+1}-\mathbf{z}^n) \ .\end{aligned} \tag{4.93}$$

In view of the directionality condition of the discrete derivative (4.80), this yields

$$H(\mathbf{z}^{n+1}) - H(\mathbf{z}^n) + \sum_{k=1}^{m}\lambda_k^{n+1}(g_{\mathbf{q}}(\mathbf{q}^{n+1}) - g_{\mathbf{q}}(\mathbf{q}^n)) + \sum_{k=1}^{m}\gamma^{n+1}(g_{\mathbf{v}}(\mathbf{z}^{n+1}) - g_{\mathbf{v}}(\mathbf{z}^n)) = 0 \ . \tag{4.94}$$

Due to the vanishing constraints (4.88c) and (4.88d), one obtains

$$H(\mathbf{z}^{n+1}) - H(\mathbf{z}^n) = 0 \ , \tag{4.95}$$

such that the Hamiltonian H, which is a conserved quantity of Hamiltonian systems, is also constant for discrete solutions provided by the EM scheme for the GGL functional. Moreover, we want to demonstrate the conservation of discrete momentum maps, as proposed in (2.105). By assumption, the momentum maps $J_{\boldsymbol{\xi}}$ of Hamiltonian systems defined in (2.40) are at most quadratic. Therefore, we are allowed to write

$$J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1}) - J_{\boldsymbol{\xi}}(\mathbf{z}^{n}) = \mathrm{D}_{\mathbf{q}} J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1/2}) \cdot (\mathbf{q}^{n+1} - \mathbf{q}^{n}) + \mathrm{D}_{\mathbf{p}} J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1/2}) \cdot (\mathbf{p}^{n+1} - \mathbf{p}^{n}) \ , \quad (4.96)$$

where $\mathrm{D}_{\mathbf{q}}(\bullet)$ and $\mathrm{D}_{\mathbf{p}}(\bullet)$ denote the exact partial derivatives (A.3). Taking into account the definition of momentum maps (2.40), which can be recast by using (2.38) as

$$\mathrm{D}_{\mathbf{q}} J_{\boldsymbol{\xi}} = -\mathbf{w}_{\boldsymbol{\xi}} \ , \quad (4.97a)$$

$$\mathrm{D}_{\mathbf{p}} J_{\boldsymbol{\xi}} = +\mathbf{v}_{\boldsymbol{\xi}} \ , \quad (4.97b)$$

we are able to proceed with

$$J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1}) - J_{\boldsymbol{\xi}}(\mathbf{z}^{n}) = -\mathbf{w}_{\boldsymbol{\xi}}(\mathbf{z}^{n+1/2}) \cdot (\mathbf{q}^{n+1} - \mathbf{q}^{n}) + \mathbf{v}_{\boldsymbol{\xi}}(\mathbf{z}^{n+1/2}) \cdot (\mathbf{p}^{n+1} - \mathbf{p}^{n}) \ . \quad (4.98)$$

Now it is possible to insert the discrete equations of motion (4.88a) and (4.88b), respectively. This eventually yields

$$J_{\boldsymbol{\xi}}(\mathbf{z}^{n+1}) - J_{\boldsymbol{\xi}}(\mathbf{z}^{n}) = -h \, \mathsf{D}^{\mathrm{G}} H(\mathbf{z}^{n}, \mathbf{z}^{n+1}) \cdot \boldsymbol{\xi}_{P}(\mathbf{z}^{n+1/2}) \ , \quad (4.99)$$

which vanishes in view of the orthogonality condition of discrete derivatives given in (4.86). As already discussed towards the ending of section 2.2, the conservation of $J_{\boldsymbol{\xi}}$ includes the fact that the angular momentum and the linear momentum are conserved quantities. As we have shown now, the EM scheme for GGL functional is capable of inheriting this property in a discrete sense such that the angular momentum is conserved in a discrete sense, viz.

$$\mathbf{L}^{n+1} - \mathbf{L}^{n} = \mathbf{0} \ . \quad (4.100)$$

4.4.4 Numerical Example: Four-Particle System

The 4-particle system - as firstly introduced by Gonzalez [14] - is investigated for a total time period of 10 s with $h = 0.05$ s with the present EM scheme. Masses have been chosen as $m_1 = 1, m_2 = 3, m_3 = 2.3, m_4 = 1.7$ and the four particles are subject to the following initial conditions:

$$\mathbf{q}_1^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \mathbf{q}_2^0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \mathbf{q}_3^0 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad , \quad \mathbf{q}_4^0 = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \quad (4.101)$$

and

$$\mathbf{p}_1^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \mathbf{p}_2^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \mathbf{p}_3^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \mathbf{p}_4^0 = \begin{bmatrix} 0 \\ 3 \\ 2 \end{bmatrix} \ . \tag{4.102}$$

For a schematic depiction of the problem see Fig. 4.19. There is no external potential and therefore no external acceleration. The internal potential of the system is governed by the two spring elements as

$$V_{\text{int}} = \frac{1}{2}\, k_1 \left((\mathbf{q}_3 - \mathbf{q}_1) \cdot (\mathbf{q}_3 - \mathbf{q}_1) - l_{13}^2 \right)^2 + \frac{1}{2}\, k_2 \left((\mathbf{q}_4 - \mathbf{q}_2) \cdot (\mathbf{q}_4 - \mathbf{q}_2) - l_{24}^2 \right)^2 \ , \tag{4.103}$$

where spring stiffnesses are set to $k_1 = 1\,\text{N/m}$ and $k_2 = 10\,\text{N/m}$ and the rest lengths are $l_{13} = l_{24} = 1\,\text{m}$, respectively. The system underlies the following two constraints on configuration level:

$$g_1^{\mathbf{q}}(\mathbf{q}) = \frac{1}{2} \left((\mathbf{q}_2 - \mathbf{q}_1) \cdot (\mathbf{q}_2 - \mathbf{q}_1) - l_{12}^2 \right) = 0 \ , \tag{4.104a}$$

$$g_2^{\mathbf{q}}(\mathbf{q}) = \frac{1}{2} \left((\mathbf{q}_4 - \mathbf{q}_3) \cdot (\mathbf{q}_4 - \mathbf{q}_3) - l_{34}^2 \right) = 0 \ . \tag{4.104b}$$

The problem has been solved with Newton's method and the corresponding tolerance has been set to $\varepsilon = 10^{-9}$. The computation has been performed using the *metis* code, which is available at [58]. The motion of the four-particle system is depicted in Fig. 4.20. The integration scheme is unconditionally stable, which has been investigated

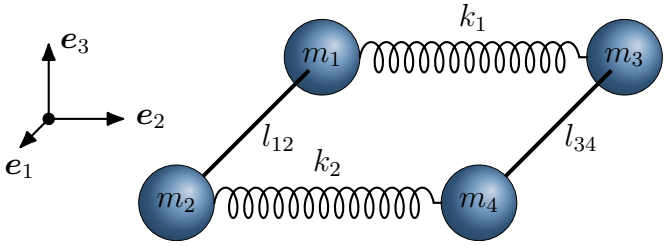

Figure 4.19: Four-particle system

with arbitrarily big values of h. This is a direct consequence of the conservation of the Hamiltonian, which is shown in Fig. 4.21. The increment in H from one time step to another is of the order of machine precision (cf. Fig. 4.23). Moreover, the EM scheme is capable of conserving the angular momentum vector in a discrete sense. We have displayed the temporal evolution of $\mathbf{L}$ in Fig. 4.22 and the increments are depicted in Fig. 4.24. By design, the constraints both on configuration and on momentum level are correctly captured (cf. 4.25 and 4.26, respectively). Thus, the EM scheme inherits crucial conservation properties of the continuous dynamical systems in a manner that leads to good approximations. However, it is to mention that EM integrators do not conserve the symplectic two-form and thus do not represent symplectic methods. In Fig. 4.27 it becomes visible that the present EM conserving scheme is second order accurate just like the classic EM integrator for constrained systems presented by Gonzalez [14]. As already done in a similar manner in Section 4.2.3 and 4.3.5, we have displayed the relative error

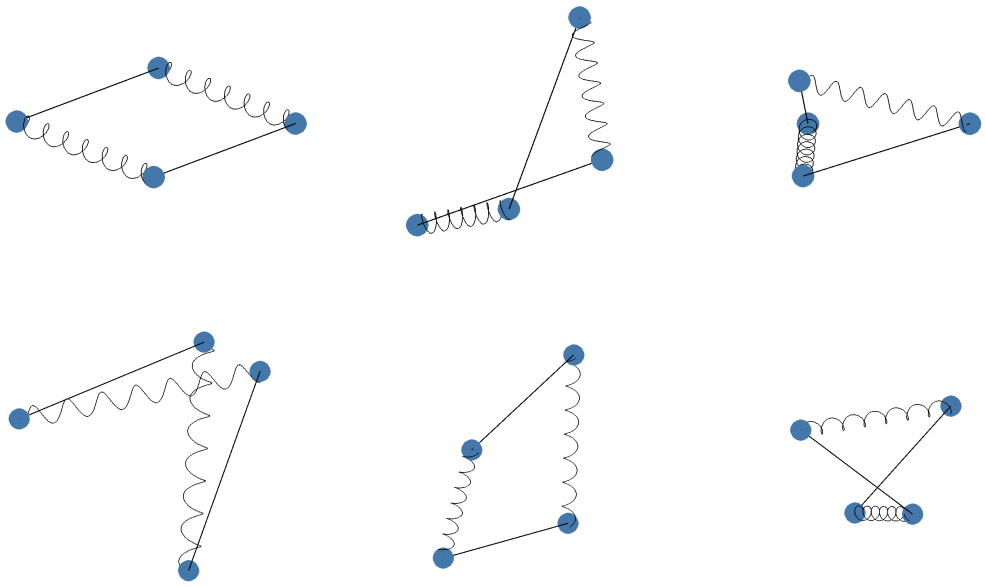

Figure 4.20: Configuration of the four-particle system at $t = \{0\,,\,2\,,\,4\,,\,6\,,\,8\,,\,10\}\,\mathrm{s}$.

for the position of the fourth particle after one second $\mathbf{q}_4(t = 1\,\mathrm{s})$ for multiple choices of the time step size h. The relative error is defined via

$$e = \frac{||\mathbf{q}_4(t = 1\,\mathrm{s}) - \mathbf{q}_{4,\mathrm{ref}}||}{||\mathbf{q}_{4,\mathrm{ref}}||}\,, \tag{4.105}$$

where $\mathbf{q}_{4,\mathrm{ref}}$ represents the solution after one second of EM scheme with secondary constraints with $h = 10^{-4}\,\mathrm{s}$.

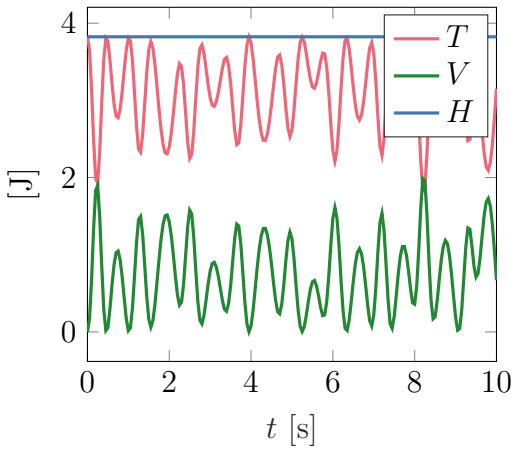

Figure 4.21: Energy quantities

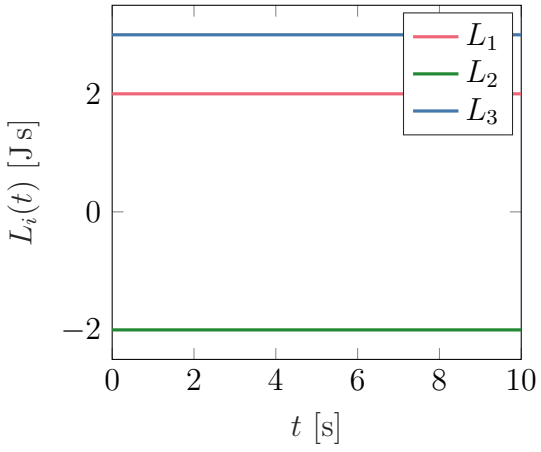

Figure 4.22: Angular momentum

As can be seen, the newly analyzed EM scheme with secondary constraints ("EMS-GGL") does not provide better approximations for the position than the originial EM scheme by Gonzalez ("EMS-std."). In fact, the difference in position is only of the order of $10^{-5}\,\mathrm{m}$ and the difference in momenta of order $10^{-3}\,\mathrm{kg\,m/s}$ for $h = 0.1\,\mathrm{s}$. The EM integrator without secondary constraints exhibits drift phenomena in the constraints on momentum level such that $\mathbf{g}^{\mathbf{v}}$ is of the order of 10^{-5}. The newly presented EM scheme is capable of capturing the secondary constraints down to machine precision (cf. Fig. 4.26) and therefore alleviates drift phenomena completely. At the same time, it has been validated that the previously used EM integrator by Gonzalez yields good approximations. For the present example it is thus admissible to deploy the simpler EM scheme without secondary constraints. However, this is not necessarily true for other problems, where the consideration of constraints on momentum level might be of greater importance.

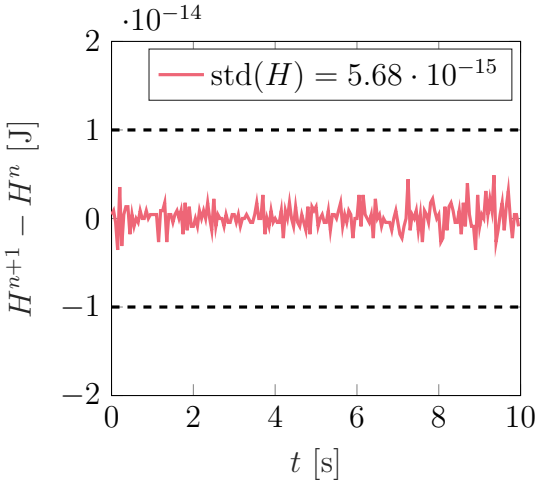

Figure 4.23: Hamiltonian difference

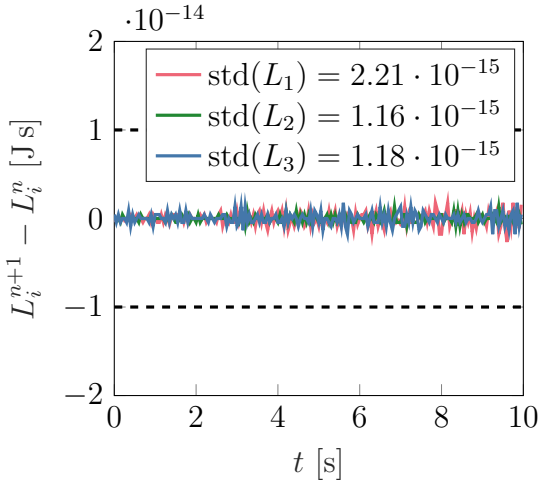

Figure 4.24: Angular momentum difference

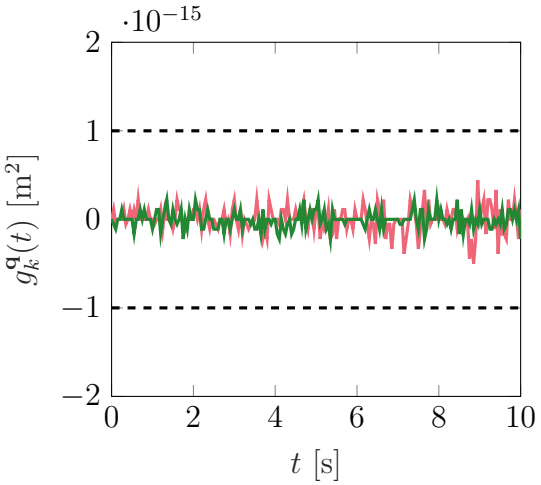

Figure 4.25: Constraints of configuration level

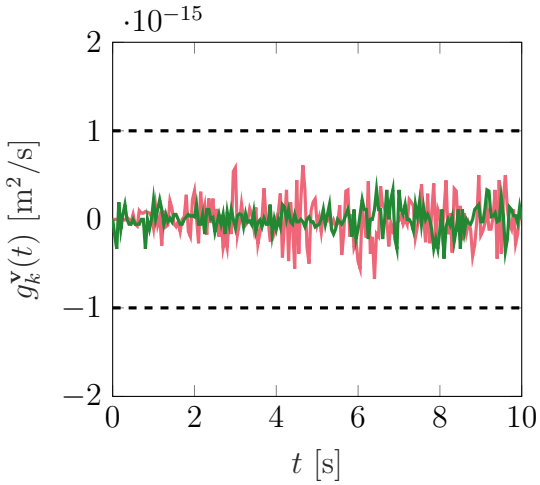

Figure 4.26: Constraints on velocity level

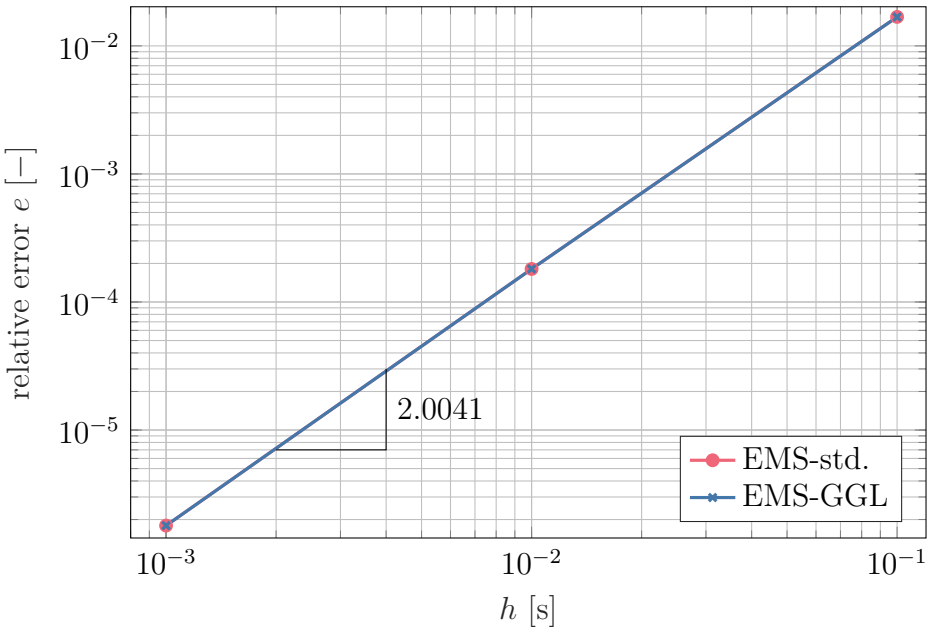

Figure 4.27: h-convergence of relative error in $\mathbf{q}$

5 Conclusion

In this thesis, a new variational principle for the analysis of constrained dynamics has been proposed (cf. Sec. 4.1). The underlying functional takes account of both primary and secondary constraints. Due to its mixed character with independent position, velocity and momentum quantities, it generalizes Livens principle [5] and thus implies Lagrangian and Hamiltonian viewpoints. By coupling constraints on position and velocity level into the equations we have obtained a set of DAEs which can be regarded as an extension of the well-known GGL stabilization [50]. Contrary to the original formulation however, the emanating equations of motion have Hamiltonian structure.

The novel GGL functional gives rise to DAEs with differentiation index 2 and thus circumvents the numerical problems of the classical constrained EL equations of constrained dynamics with index 3. We could show, that the formulation is symplectic and has Hamiltonian structure. The conservation principles of constrained dynamics can be carried over to the novel augmented formulation. We have demonstrated that in the time-continuous case the additional Lagrange multipliers need to vanish such that the classical formulation [50] is included into the newly proposed variational principle. However, in contrast to the originial formulation, this property is not required to achieve the conservation of the Hamiltonian and the symplectic structure.

Based on this novel formalism, we have succesfully derived two kinds of variational integrators. The first one is a straightforward generalization of the symplectic Euler method for constrained systems (cf. Sec. 4.2). Both primary and secondary constraints are captured exactly. Unfortunately, this method does not inherit the symplectic structure of constrained dynamics and the angular momentum is not preserved along the solutions of the corresponding DEL. Typically, variational integrators are said to be symplectic and conserve the momentum maps of the dynamic system (cf. Marsden et al. [19]). Thus, further research should investigate the reasons why this first variational integrator is not symplectic and how this property can be achieved.

In a next step we have chosen a more sophisticated approach by making use of auxiliary position and momentum quantities inspired by Betsch et al. [25] (cf. Sec. 4.3). Consequently, a two-parameter one-stage method has been derived as a variational integrator. Contrary to the first approximation, this scheme is actually symplectic and conserves the momentum maps of the dynamical system. Depending on the evaluation of the constraint function we have distinguished between two types of integration schemes. Option A unfortunately could neither conserve primary nor secondary constraints in discrete time steps. Howevever, a midpoint evaluation could be regarded as an application of the midpoint rule to the EL equations of the novel variational principle and thus yielded a second order accurate approximation. Option B, which is based on a

trapezoidal evaluation of the constraints on position level, fulfilled both level constraints in discrete time-steps. This choice unfortunately exhibits only a first-order convergence of position errors. It achieves an approximately equal performance to already existing methods but has the advantage of capturing the secondary constraints.

Towards the end of this work, we have covered an energy-momentum conserving scheme based on the concept of discrete derivatives (cf. Sec. 4.4). This procedure has been admissible since the equations of motion of the new variational principle have Hamiltonian structure. By design, this scheme conserves the phase space, the momentum maps and the Hamiltonian but not the symplectic two-form. This scheme can be regarded as an extension of the EM schemes by Gonzalez [14]. However, it captures also the constraints on momentum level and thus achieves a more realistic approximation of the physical processes. We could observe, that for the chosen numerical example, the additional Lagrange multipliers are significantly small and the new scheme performs equally well as the original EM integrator for constrained systems. In future works, it can be of interest to investigate, whether the extended version might be beneficial in other applications. One drawback of EM schemes in general is the implicit form of the equations of motion. For highly dynamical systems in particular, it might be advantageous to use explicit methods combined with small time step sizes h. However EM schemes are numerically very stable and yield a good approximation quality. Thus, the newly proposed formulation has gained more realistic results than existing schemes.

We have shown that the novel variational framework represents a promising basis for the construction of structure-preserving integration schemes. The methods which have been deduced throughout this work can thus be seen as a starting point for further approaches. Therefore, the future objectives can be the design of further variational integrators that capture the crucial properties as symplecticness, momentum conservation and fulfillment of both primary and secondary constraints. In particular, the construction of an one-stage variational integrator with second order accuracy is yet unachieved.

For the search of further structure-preserving integrators based on the GGL functional, one might focus on the construction of higher order methods. Therefore, two different approaches are promising: Firstly, partioned Runge Kutta schemes that can be gained as variational integrators from Livens principle could be generalized with respect to constrained dynamics. The work by Bou-Rabee [7] might serve as a starting point. Secondly, one might aim for Galerkin-based methods for constrained systems corresponding to already existing works by Ober-Blöbaum [62], Ober-Blöbaum et al. [63] and Wenger et al. [29]. Another promising idea is the application of continuous Galerkin schemes for index 2 DAEs to the novel functional for constrained dynamics. Altmann et al. [64] have recently provided a corresponding framework.

Altogether, the newly proposed Livens-based framework has yielded promising results for a variational consideration of both primary and secondary constraints in the field of dynamics. The results of this work bode well for the succesful search of further structure-preserving integrators. The novel variational principle opens up a plethora of new integration schemes which can provide more realistic simulations of dynamical systems subject to holonomic constraints.

Appendix A

Mathematical Aspects

A.1 Mathematical Operators

Throughout this thesis multiple differential operations are employed. The following part gives the respective definitions and describes the notations used in the present work. For more details we refer to the monograph by Itskov [65].

Let $\mathcal{F}$ be a smooth scalar, vector or tensor valued field depending on $\mathbf{x} \in \mathbb{R}^d$. Then, the derivative with respect to time is denoted as a dotted expression

$$\dot{\mathcal{F}} = \frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} \ . \tag{A.1}$$

Moreover, the gradient operator with respect to $\mathbf{x}$ is given by

$$\mathrm{D}\mathcal{F}(\mathbf{x}) = \operatorname{grad} \mathcal{F}(\mathbf{x}) = \frac{\mathrm{d}\mathcal{F}}{\mathrm{d}\mathbf{x}} \ . \tag{A.2}$$

If we assume a multi-variable field $\mathcal{F}(\mathbf{x}, \mathbf{y})$ with $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ we can introduce the partial derivatives as

$$\mathrm{D}_1\mathcal{F}(\mathbf{x}, \mathbf{y}) = \mathrm{D}_{\mathbf{x}}\mathcal{F}(\mathbf{x}, \mathbf{y}) = \frac{\partial \mathcal{F}}{\partial \mathbf{x}} \ , \tag{A.3a}$$

$$\mathrm{D}_2\mathcal{F}(\mathbf{x}, \mathbf{y}) = \mathrm{D}_{\mathbf{y}}\mathcal{F}(\mathbf{x}, \mathbf{y}) = \frac{\partial \mathcal{F}}{\partial \mathbf{y}} \ , \tag{A.3b}$$

where the respective argument is indicated either by its position or the quantity appears as a subscript. Furthermore, the second-order derivative of a field is denoted by

$$\mathrm{D}^2\mathcal{F}(\mathbf{x}) = \frac{\mathrm{d}^2\mathcal{F}}{\mathrm{d}\mathbf{x}^2} \ . \tag{A.4}$$

Assuming a scalar field $f(\mathbf{x}, \mathbf{y})$, which is at least twice differentiable, the second-order partial derivatives adressed via the arguments position as well, such that exemplarily

$$\mathrm{D}^2_{12} f(\mathbf{x}, \mathbf{y}) = \frac{\partial^2 f(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x} \partial \mathbf{y}} \ . \tag{A.5}$$

All second-order partial derivatives can be comprised within the *Hessian* matrix of f

$$\mathrm{D}^2 f(\mathbf{x},\mathbf{y}) = \begin{bmatrix} \mathrm{D}^2_{11} f(\mathbf{x},\mathbf{y}) & \mathrm{D}^2_{12} f(\mathbf{x},\mathbf{y}) \\ \mathrm{D}^2_{21} f(\mathbf{x},\mathbf{y}) & \mathrm{D}^2_{22} f(\mathbf{x},\mathbf{y}) \end{bmatrix} = \mathrm{D}^2 f(\mathbf{x},\mathbf{y})^{\mathrm{T}} \ , \tag{A.6}$$

which is a symmetric block matrix due to *Schwarz's theorem* on second-order partial derivatives for scalar fields

$$\frac{\partial^2 f}{\partial x_i \partial y_j} = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial y_j}\right) = \frac{\partial}{\partial y_j}\left(\frac{\partial f}{\partial x_i}\right) = \frac{\partial^2 f}{\partial y_j \partial x_i} \ . \tag{A.7}$$

Consequently, $\mathrm{D}^2_{11} f(\mathbf{x},\mathbf{y})$ and $\mathrm{D}^2_{22} f(\mathbf{x},\mathbf{y})$ are symmetric matrices themselves and the off-diagonal entries satisfy $\mathrm{D}^2_{ij} f(\mathbf{x},\mathbf{y}) = \mathrm{D}^2_{ji} f(\mathbf{x},\mathbf{y})^{\mathrm{T}}$. For the purpose of variational principles of dynamics, we make use of variational calculus multiple times. The first variation of a field is given by

$$\delta\mathcal{F}(\mathbf{x}) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{F}(\mathbf{x}+\varepsilon\delta\mathbf{x})\Big|_{\varepsilon=0} = \mathrm{D}\mathcal{F}(\mathbf{x})\delta\mathbf{x} \ , \tag{A.8}$$

which represents a directional derivative along $\delta\mathbf{x}$. Note, that we denote a matrix-vector multiplication of any matrix $\mathbf{A} \in \mathbb{R}^{d\times d}$ with a vector $\mathbf{b} \in \mathbb{R}^d$ in the sense of a linear map as $\mathbf{A}\,\mathbf{b}$. For scalar fields f, this directional derivative is given by the scalar product between the gradient of f and $\delta\mathbf{x}$, viz.

$$\delta f(\mathbf{x}) = \mathrm{D}f(\mathbf{x}) \cdot \delta\mathbf{x} \ . \tag{A.9}$$

For multi-variable fields, we obtain

$$\delta\mathcal{F}(\mathbf{x},\mathbf{y}) = \mathrm{D}_1\mathcal{F}(\mathbf{x},\mathbf{y})\delta\mathbf{x} + \mathrm{D}_2\mathcal{F}(\mathbf{x},\mathbf{y})\delta\mathbf{y} \ . \tag{A.10}$$

For the analysis of numerical investigation we also deploy the standard deviation

$$\mathrm{std}(\Phi) = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N} |\Phi_i - \bar{\Phi}|^2} \tag{A.11}$$

of a quantity Φ where N denotes the number of measurements and $\bar{\Phi}$ is the mean value of Φ such that

$$\bar{\Phi} = \frac{1}{N}\sum_{i=1}^{N} \Phi_i \ . \tag{A.12}$$

A.2 Properties of the Wedge Product

For differential one-forms, given in vector notation as $\mathrm{d}\mathbf{a}, \mathrm{d}\mathbf{b}$ and $\mathrm{d}\mathbf{c} \in \mathbb{R}^d$, any scalar valued quantities $\alpha, \beta \in \mathbb{R}$, any matrix $\mathbf{A} \in \mathbb{R}^{d\times d}$ and any symmetric matrix $\mathbf{B} = \mathbf{B}^{\mathrm{T}} \in \mathbb{R}^{d\times d}$ the wedge product defined in (2.83) has the following properties according to Leimkuhler et al. [12]:

1. *Skew-symmetry*:

$$\mathrm{d}\mathbf{a} \wedge \mathrm{d}\mathbf{b} = -\,\mathrm{d}\mathbf{b} \wedge \mathrm{d}\mathbf{a} \;, \tag{A.13a}$$

   which directly implies

$$\mathrm{d}\mathbf{a} \wedge \mathrm{d}\mathbf{a} = 0 \;. \tag{A.13b}$$

2. *Bilinearity*:

$$\mathrm{d}\mathbf{a} \wedge (\alpha\ \mathrm{d}\mathbf{b} + \beta\,\mathrm{d}\mathbf{c}) = \alpha\,\mathrm{d}\mathbf{a} \wedge \mathrm{d}\mathbf{b} + \beta\,\mathrm{d}\mathbf{a} \wedge \mathrm{d}\mathbf{c} \;. \tag{A.14}$$

3. *Rule of matrix multiplication*:

$$\mathrm{d}\mathbf{a} \wedge (\mathbf{A}\,\mathrm{d}\mathbf{b}) = (\mathbf{A}^{\mathrm{T}}\,\mathrm{d}\mathbf{a}) \wedge \mathrm{d}\mathbf{b} \;, \tag{A.15}$$

   which follows directly from the definition (2.83) and usage of the bilinearity property (A.14).

4. *Rule of symmetric matrix multiplication*:

$$\mathrm{d}\mathbf{a} \wedge (\mathbf{B}\,\mathrm{d}\mathbf{a}) = 0 \;. \tag{A.16}$$

   This useful rule can be gained by applying the properties (A.15) and (A.13).

Appendix B

Symplecticness of the One-stage Methods

In order to gain (4.41) the procedure is as follows: Firstly we will take the differential equations of the discrete equations of motion given in (4.38a) - (4.38d) making use of (4.37) as:

$$\mathrm{d}\mathbf{q}^{n+1} - \mathrm{d}\mathbf{q}^{n} = \mathrm{D}_1\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{q}^{n} + \mathrm{D}_1\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{q}^{n+1} + \mathrm{D}_3\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{v}^{n} + \mathrm{D}_{\boldsymbol{\gamma}}\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\boldsymbol{\gamma}^{n}\ , \tag{B.1a}$$

$$\begin{aligned}\mathrm{d}\mathbf{p}^{n+1} - \mathrm{d}\mathbf{p}^{n} + \mathrm{d}\mathbf{P}^{n} = {}& \mathrm{D}^2_{11}L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{q}^{n} + \mathrm{D}^2_{12}L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{q}^{n+1} + \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_1L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\boldsymbol{\lambda}^{n}\\ & - (\mathrm{D}^2_{11}\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{q}^{n} + \mathrm{D}^2_{12}\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{q}^{n+1})^{\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^{n})\\ & - \mathrm{D}_{\boldsymbol{\gamma}}(\mathrm{D}_1\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^{n}))\,\mathrm{d}\boldsymbol{\gamma}^{n} - \mathrm{D}_1\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n})\ ,\end{aligned} \tag{B.1b}$$

$$\begin{aligned}-\mathrm{d}\mathbf{P}^{n} = {}& \mathrm{D}^2_{21}L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{q}^{n} + \mathrm{D}^2_{22}L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{q}^{n+1} + \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_2L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\boldsymbol{\lambda}^{n}\\ & - (\mathrm{D}^2_{12}\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{q}^{n} + \mathrm{D}^2_{22}\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\mathbf{q}^{n+1})^{\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^{n})\\ & - \mathrm{D}_{\boldsymbol{\gamma}}(\mathrm{D}_2\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^{n}))\,\mathrm{d}\boldsymbol{\gamma}^{n} - \mathrm{D}_2\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n})\ ,\end{aligned} \tag{B.1c}$$

$$\mathbf{0} = \mathrm{D}^2_{33}L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{v}^{n+1} - \mathrm{D}_3\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n})\ . \tag{B.1d}$$

Note that in the last equation we may assume that $L_\mathrm{d}^{\boldsymbol{\lambda}}$ once differentiated with respect to $\mathbf{v}^{n+1}$ does not depend on any other argument anymore. Moreover we assume that $\mathrm{D}_3\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}$ is constant. Next the following apropriate wedge products are computed: Computing $(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n}) \wedge$ (B.1a) yields

$$\begin{aligned}& - (\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n}) \wedge \mathrm{d}\mathbf{q}^{n} - \mathrm{D}_1\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n}) \wedge \mathrm{d}\mathbf{q}^{n}\\ & + \mathrm{d}\mathbf{P}^{n} \wedge \mathrm{d}\mathbf{q}^{n+1} - \mathrm{D}_2\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n}) \wedge \mathrm{d}\mathbf{q}^{n+1} + \mathrm{d}\mathbf{p}^{n+1} \wedge \mathrm{d}\mathbf{q}^{n+1}\\ & \qquad = (\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n}) \wedge \mathrm{D}_{\boldsymbol{\gamma}}\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}}\,\mathrm{d}\boldsymbol{\gamma}^{n}\ ,\end{aligned} \tag{B.2}$$

where (B.1d) has been taken into account and the symmetric matrix multiplication property of the wedge product (A.16) has been used such that

$$\mathrm{D}_3\mathbf{f}_\mathrm{d}^{\boldsymbol{\gamma}\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \mathrm{d}\mathbf{P}^{n}) \wedge \mathrm{d}\mathbf{v}^{n+1} = \mathrm{D}^2_{33}L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{v}^{n+1} \wedge \mathrm{d}\mathbf{v}^{n+1} = \mathbf{0}\ . \tag{B.3}$$

Taking the wedge product (B.1b) $\wedge\, \mathrm{d}\mathbf{q}^n$ leads to the relationship

$$\begin{aligned}(\,\mathrm{d}\mathbf{p}^{n+1} + \,\mathrm{d}\mathbf{P}^n + \mathrm{D}_1\mathbf{f}_\mathrm{d}^{\gamma\,\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \,\mathrm{d}\mathbf{P}^n) - \,\mathrm{d}\mathbf{p}^n) \wedge \,\mathrm{d}\mathbf{q}^n \\ = \mathrm{D}_{12}^2 L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{q}^{n+1} \wedge \,\mathrm{d}\mathbf{q}^n + \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_1 L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\boldsymbol{\lambda}^n \wedge \,\mathrm{d}\mathbf{q}^n \\ - (\mathrm{D}_{12}^2 \mathbf{f}_\mathrm{d}^{\gamma}\,\mathrm{d}\mathbf{q}^{n+1})^\mathrm{T}(\mathbf{p}^{n+1} + \mathbf{P}^n) \wedge \,\mathrm{d}\mathbf{q}^n - \mathrm{D}_\gamma(\mathrm{D}_1\mathbf{f}_\mathrm{d}^{\gamma\,\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^n))\,\mathrm{d}\boldsymbol{\gamma}^n \wedge \,\mathrm{d}\mathbf{q}^n\,,\end{aligned} \tag{B.4}$$

where (A.16) has been used once more. The product (B.1c) $\wedge\, \mathrm{d}\mathbf{q}^{n+1}$ can be rewritten as

$$\begin{aligned}(-\,\mathrm{d}\mathbf{P}^n + \mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma\,\mathrm{T}}(\,\mathrm{d}\mathbf{p}^{n+1} + \,\mathrm{d}\mathbf{P}^n)) \wedge \,\mathrm{d}\mathbf{q}^{n+1} \\ = \mathrm{D}_{21}^2 L_\mathrm{d}^{\boldsymbol{\lambda}}\,\mathrm{d}\mathbf{q}^n \wedge \,\mathrm{d}\mathbf{q}^{n+1} + \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_2 L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\boldsymbol{\lambda}^n \wedge \,\mathrm{d}\mathbf{q}^{n+1} \\ - (\mathrm{D}_{21}^2 \mathbf{f}_\mathrm{d}^{\gamma}\,\mathrm{d}\mathbf{q}^{n+1})^\mathrm{T}(\mathbf{p}^{n+1} + \mathbf{P}^n) \wedge \,\mathrm{d}\mathbf{q}^{n+1} \\ - \mathrm{D}_\gamma(\mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma\,\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^n))\,\mathrm{d}\boldsymbol{\gamma}^n \wedge \,\mathrm{d}\mathbf{q}^{n+1}\,.\end{aligned} \tag{B.5}$$

Summation of the previous Eqns. (B.2), (B.4) and (B.5) is quite handy since several terms cancel out. We obtain

$$\begin{aligned}-\,\mathrm{d}\mathbf{p}^n \wedge \,\mathrm{d}\mathbf{q}^n + \,\mathrm{d}\mathbf{p}^{n+1} \wedge \,\mathrm{d}\mathbf{q}^{n+1} \\ = \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_1 L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\boldsymbol{\lambda}^n \wedge \,\mathrm{d}\mathbf{q}^n - \mathrm{D}_\gamma(\mathrm{D}_1\mathbf{f}_\mathrm{d}^{\gamma\,\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^n))\,\mathrm{d}\boldsymbol{\gamma}^n \wedge \,\mathrm{d}\mathbf{q}^n \\ + \mathrm{D}_{\boldsymbol{\lambda}}(\mathrm{D}_2 L_\mathrm{d}^{\boldsymbol{\lambda}})\,\mathrm{d}\boldsymbol{\lambda}^n \wedge \,\mathrm{d}\mathbf{q}^{n+1} - \mathrm{D}_\gamma(\mathrm{D}_2\mathbf{f}_\mathrm{d}^{\gamma\,\mathrm{T}}(\mathbf{p}^{n+1} + \mathbf{P}^n))\,\mathrm{d}\boldsymbol{\gamma}^n \wedge \,\mathrm{d}\mathbf{q}^{n+1} \\ + (\,\mathrm{d}\mathbf{p}^{n+1} + \,\mathrm{d}\mathbf{P}^n) \wedge \mathrm{D}_\gamma\mathbf{f}_\mathrm{d}^{\gamma}\,\mathrm{d}\boldsymbol{\gamma}^n\,,\end{aligned} \tag{B.6}$$

where we can apply the skew-symmetry property of the wedge product (A.13) on the left hand side and on the right hand side it is possible to make us of the matrix multiplication property (A.15) such that $\mathrm{d}\boldsymbol{\lambda}^n$ and $\mathrm{d}\boldsymbol{\gamma}^n$ can be collected. Eventually we arrive at the relationship (4.41). Taking into account the differential forms of the discrete constraint equations the right hand site can be made zero, as shown in Section 4.3.2.

Appendix C

Alternative One-stage Theta Methods

C.1 Option A with Midpoint Evaluation

The discrete equations of motion (4.62) of the symplectic theta integrator with a trapezoidal evaluation of the constraint equation where the parameters are chosen as $\theta = \vartheta = 0.5$ read

$$\mathbf{q}^{n+1} - \mathbf{q}^{n} = h\,\mathbf{v}^{n+1} + h\,\mathbf{M}^{-1}\mathbf{G}(\mathbf{q}^{n+1/2})^{\mathrm{T}}\boldsymbol{\gamma}^{n}\ , \tag{C.1a}$$

$$\begin{aligned}\mathbf{p}^{n+1} - \mathbf{p}^{n} = {} & \mathrm{D}_1 L_{\mathrm{d}}(\mathbf{q}^{n+1/2}, \mathbf{v}^{n+1}) - \frac{h}{2}\left(\mathbf{G}(\mathbf{q}^{n}) + \mathbf{G}(\mathbf{q}^{n+1})\right)^{\mathrm{T}}\boldsymbol{\lambda}^{n} \\ & - h\sum_{k=1}^{m}\gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^{n+1/2})\mathbf{v}^{n+1}\ ,\end{aligned} \tag{C.1b}$$

$$\mathbf{M}\mathbf{v}^{n+1} = \mathbf{p}^{n+1/2} - \frac{h}{4}\left[\mathbf{G}(\mathbf{q}^{n})^{\mathrm{T}} - \mathbf{G}(\mathbf{q}^{n+1})^{\mathrm{T}}\right]\boldsymbol{\lambda}^{n}\ , \tag{C.1c}$$

$$\mathbf{g}(\mathbf{q}^{n+1/2}) = \mathbf{0}\ , \tag{C.1d}$$

$$\mathbf{G}(\mathbf{q}^{n+1/2})\mathbf{v}^{n+1} = \mathbf{0}\ . \tag{C.1e}$$

For the sake of comparability we investigated once more the steady precession of a gyroscopic top with the same simulation circumstances as in Section 4.3.5 and again with $h = 0.001\,\mathrm{s}$. By design, the constraints both on configuration level and on velocity level are not fullfilled identically anymore.

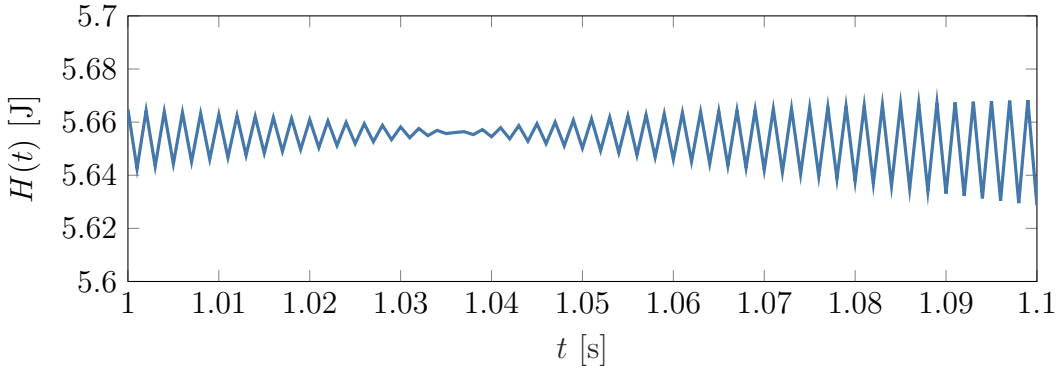

Figure C.1: $H(t)$ for $t \in [1.0\,\mathrm{s}\ ,\ 1.1\,\mathrm{s}]$

However, this choice of parameters reduces the symplectic energy oscillations with respect to $\theta = 1$ and $\vartheta = 0.5$ as can be seen in Fig. C.2. Obviously, the oscillatory behaviour of symplectic methods is present also for this choice of parameters (cf. Fig. C.1).

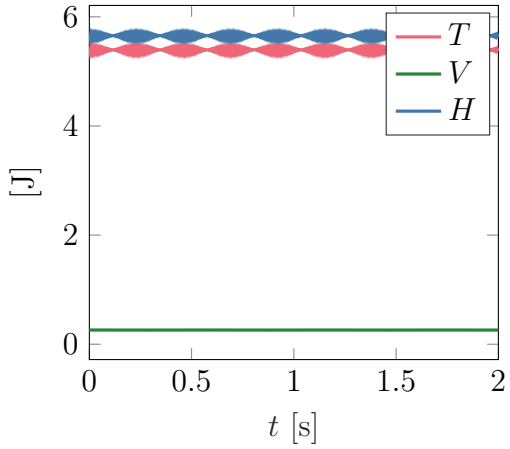

Figure C.2: Energy quantities

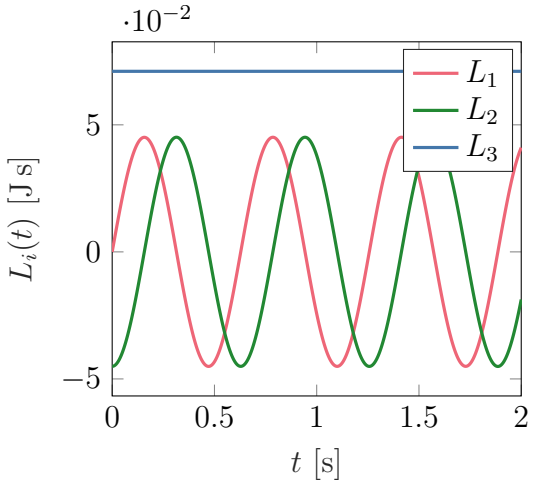

Figure C.3: Angular momentum

This also leads to an improved stability as the biggest timestep size possible without causing numerical energy pile ups could be increased from $h = 0.003125\,\mathrm{s}$ to $h = 0.0125\,\mathrm{s}$ for the gyroscopic top example. The increments in H from one time step to another is depicted in Fig. C.4. Compared to the method from Section 4.3.4 the standard deviation of H could be reduced.

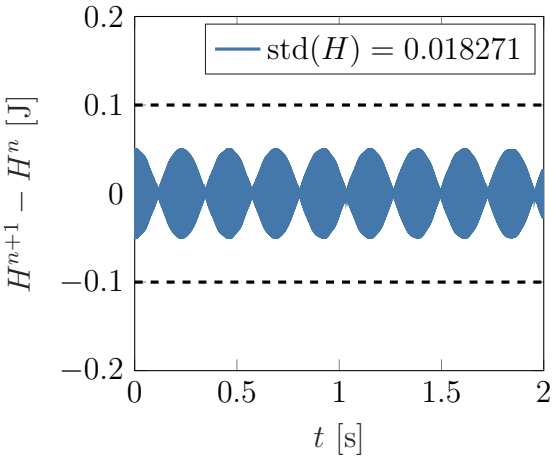

Figure C.4: Hamiltonian difference

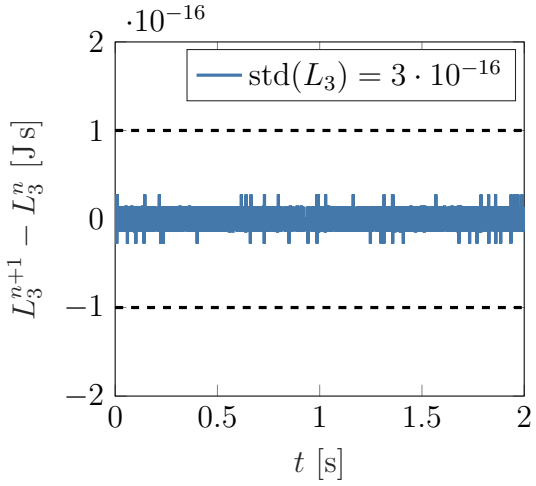

Figure C.5: Angular momentum difference

As it can be seen in Fig. C.3 the conservation of angular momentum has been captured well and increments $L_3^{n+1} - L_3^n$ are numerically zero (cf. Fig. C.5). Fig. C.6 and Fig. C.7 display the violation of primary and secondary constraints, respectively. Note that the method captures the precession height of the top better than the integrator based on option A (cf. Fig. C.8 and see Fig. 4.10 for comparison), which might be a consequence of

the reduced energy oscillations. As we have already displayed in Fig. 4.18 the symplectic one-stage theta method based on option A is second order accurate in the positions which might be due to the midpoint evaluations.

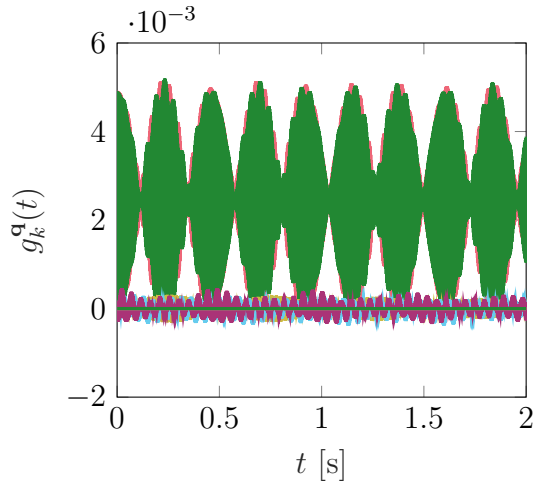

Figure C.6: Constraints on position level

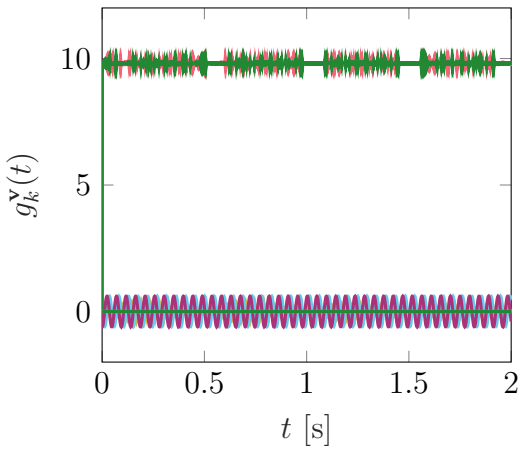

Figure C.7: Constraints on velocity level

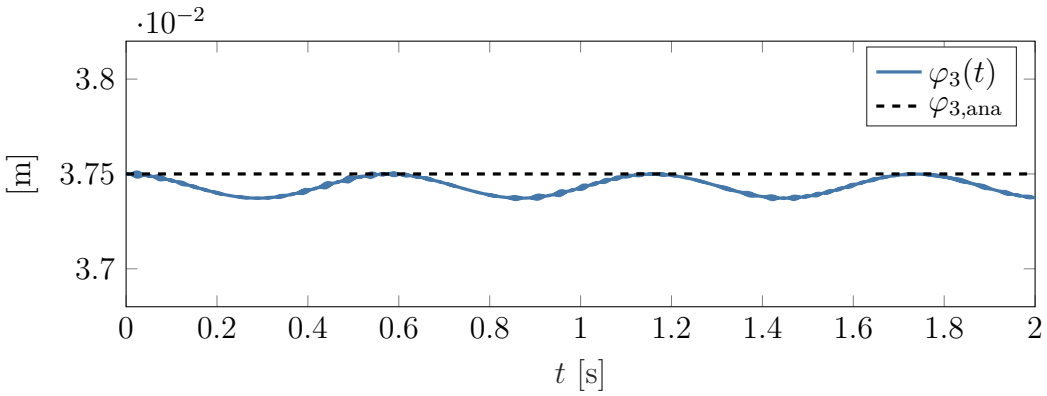

Figure C.8: Vertical coordinate of center of mass

C.2 Modified Theta Integrator

In Section 4.3.4 we have introduced a family of variational integrators based on a discrete action integral (4.34) together with an intermediate evaluation of the primary constraint (4.59). This eventually yields DEL that violate both constraints on configuration and on velocity level (cf. (4.62d) and (4.62e)). We will now replace those algebraic expression by endpoint evaluations such that the modified theta integrator is governed by

$$\mathbf{q}^{n+1} - \mathbf{q}^n = h\,\mathbf{v}^{n+1} + h\,\mathbf{M}^{-1}\mathbf{G}(\mathbf{q}^{n+\theta})^{\mathrm{T}}\boldsymbol{\gamma}^n \,, \tag{C.2a}$$

$$\mathbf{p}^{n+1} - \mathbf{p}^n = \mathrm{D}_1 L_{\mathrm{d}}(\mathbf{q}^{n+\theta}, \mathbf{v}^{n+1}) - h\,\mathbf{G}(\mathbf{q}^{n+\theta})^{\mathrm{T}}\boldsymbol{\lambda}^n - h\sum_{k=1}^{m}\gamma_k^n \mathrm{D}^2 g_k(\mathbf{q}^{n+\theta})\mathbf{v}^{n+1} \,, \tag{C.2b}$$

$$\mathbf{M}\mathbf{v}^{n+1} = \mathbf{p}^{n+1-\theta} \,, \tag{C.2c}$$

$$\mathbf{g}(\mathbf{q}^{n+1}) = \mathbf{0} \,, \tag{C.2d}$$

$$\mathbf{G}(\mathbf{q}^{n+1})\mathbf{M}^{-1}\mathbf{p}^{n+1} = \mathbf{0} \,, \tag{C.2e}$$

for $n = 0, ..., N-1$. For $\theta = 0.5$ this scheme can be interpreted as a midpoint-approximation of the differential equations (4.6a) and (4.6b), after eliminating the velocities, together with an endpoint evalutation of the primary and secondary constraints (4.6d) and (4.6e). Due to the modification in the constraints, the method is not symplectic anymore but conserves the constraint phase space $\mathcal{P}_{\mathrm{c}}$. As a consequence of the midpoint evaluation one obtains a second order scheme, which is identical to the EM scheme from Sec. 4.4.2 for systems with at most quadratic potential functions $V(\mathbf{q})$.

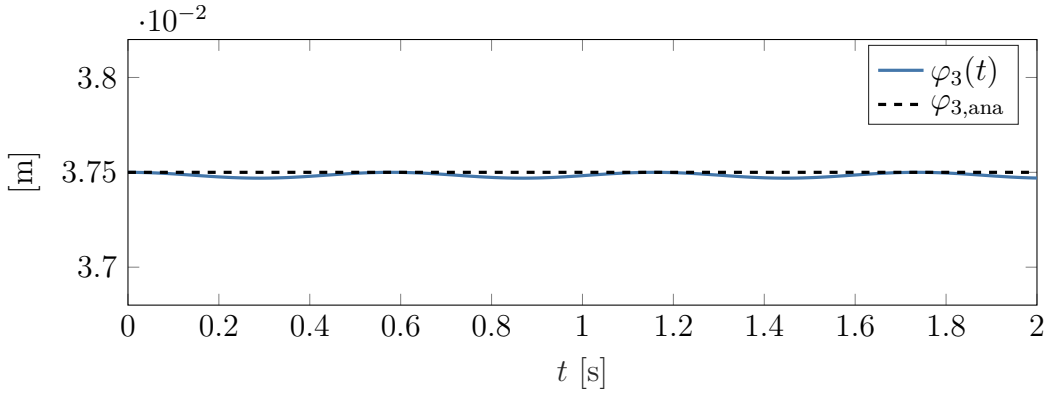

Figure C.9: Vertical coordinate of center of mass

Let us now once more investigate the steady precession of a gyroscopic top with the same simulation circumstances as in Section 4.3.5 and again with $h = 0.001\,\mathrm{s}$. Due to the given modifications, the constraints both on configuration level and on velocity level are fullfilled identically. As another consequence, symplectic energy oscillations vanish and the Hamiltonian is conserved numerically, as it can be seen in Fig. C.10. The increment $H^{n+1} - H^n$ is numerically zero (cf. Fig. C.12). The modified theta integrator is moreover very robust as the biggest timestep size possible without causing numerical energy pile ups could be increased to $h = 0.025\,\mathrm{s}$ for the gyroscopic top example.

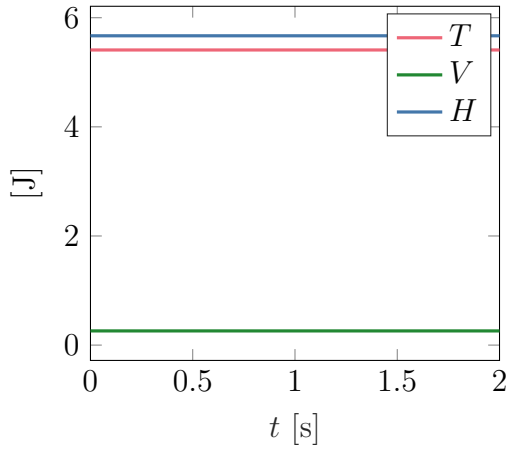

Figure C.10: Energy quantities

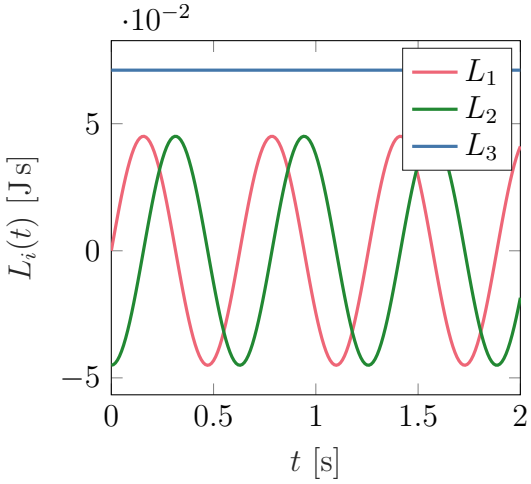

Figure C.11: Angular momentum

As it can be seen in Fig. C.3 the conservation of angular momentum has been captured well and increments $L_3^{n+1} - L_3^n$ are numerically zero (cf. Fig. C.13). Fig. C.14 and Fig. C.15 verify that primary and secondary constraints, respectively, are correctly captured. Note that the method captures the precession height of the top better than the variational integrators based on option A or B (cf. Fig. C.9), which might be a consequence of the reduced energy oscillations and the exact preservation of the phase space. As we have already displayed in Fig. 4.18 the modified theta integrator is, just like the symplectic one-stage theta method based on option A, second order accurate in the positions which might be due to the midpoint evaluations.

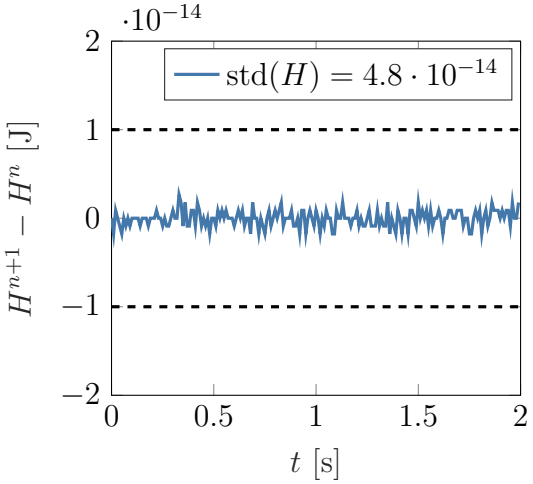

Figure C.12: Hamiltonian difference

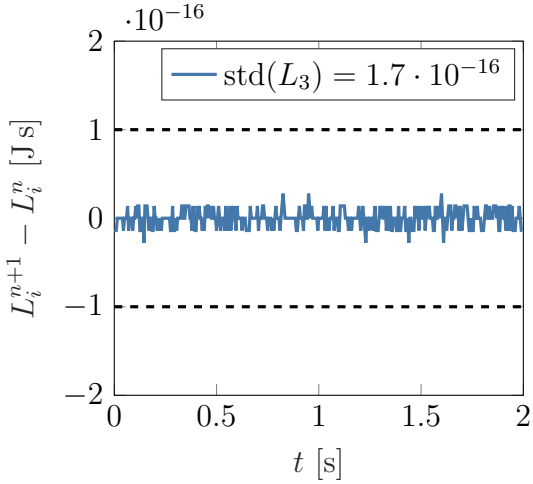

Figure C.13: Angular momentum difference

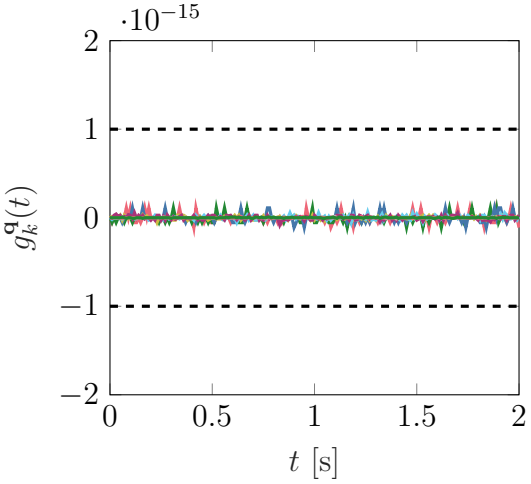

Figure C.14: Constraints on position level

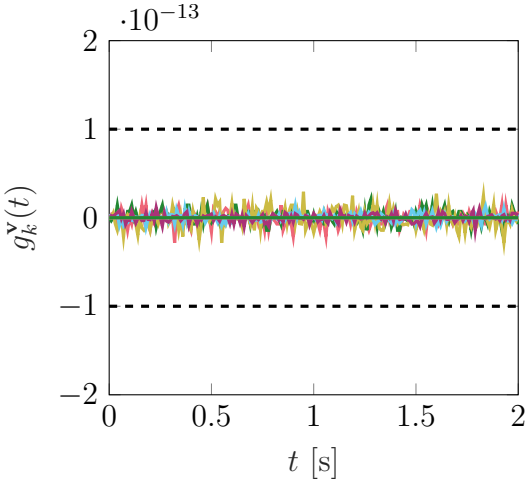

Figure C.15: Constraints on velocity level

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