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Construction and analysis of higher order variational integrators for dynamical systems with holonomic constraints

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Abstract In this work, variational integrators of higher order for dynamical systems with holonomic constraints are constructed and analyzed. The construction is based on approximating the configuration and the Lagrange multiplier via different polynomials. The splitting of the augmented Lagrangian in two parts enables the use of different quadrature formulas to approximate the integral of each part. Conditions are derived that ensure the linear independence of the higher order constrained discrete Euler-Lagrange equations and stiff accuracy. Time reversibility is investigated for the discrete flow on configuration level only as for the flow on configuration and momentum level. The fulfillment of the hidden constraints plays an important role for the time reversibility of the presented integrators. The order of convergence is investigated numerically. Order reduction of the momentum and the Lagrange multiplier compared to the order of the configuration occurs in general, but can be avoided by fulfilling the hidden constraints in a simple post processing step. Regarding efficiency versus accuracy a numerical analysis yields that higher orders increase the accuracy of the discrete solution substantially while the computational costs decrease. A comparison to the constrained Galerkin methods in Marsden and West (Acta Numerica **10**: 357–514 2001) and the symplectic SPARK integrators of Jay (SIAM Journal on Numerical Analysis **45(5)**: 1814–1842 2007) reveals that the approach presented here is more general and thus allows for more flexibility in the design of the integrator.

Keywords Variational integrators · Higher order integration · Holonomic constraints · Symplectic momentum methods · Time reversibility · Numerical convergence analysis

Mathematics Subject Classification (2000) 65L80 · 65P10 · 70F20 · 70Hxx

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1 Introduction

Variational integrators are of high interest in numerical integration theory as they inherit specific properties of the underlying mechanical system. The variational integrators base on a discrete version of the variational principle in Lagrangian mechanics. They are symplectic, momentum preserving, and show excellent long time behaviour [17]. Special interest lies in variational integrators of higher order to achieve accurate discretization schemes in conjunction with moderate computational costs. To get higher orders, one possibility is to approximate the continuous curves via polynomials of higher degrees and to use quadrature formulas of higher order for the approximation of the action integral. In the unconstrained case, this approach is a particular case of the Galerkin variational integrators, studied, e.g., in [17] and developed further and analyzed in [20] and [19].

Considering a Lagrangian system with holonomic constraints, the motion is described by index 3 differential-algebraic equations (DAEs). In the DAEs, the Lagrange multipliers λ are related to the constraint forces that prevent the system from deviation of the constraint manifold. The numerical treatment of the Lagrange multiplier and the constraints is challenging and affects the order of the approximation. Instead of discretizing the DAE directly, e.g., in [4], [8], [3], [9], a variational integrator is based on a discrete version of the variational principle also taking account of the holonomic constraints. One possibility is to approximate the holonomic constraints by stiff restraints as in [24] where a variational and linearly implicit integrator is investigated. In [17], the constrained Galerkin methods are presented as a straightforward expansion of the former mentioned Galerkin variational integrators using Lagrange multipliers. They are equivalent to constrained symplectic partitioned Runge-Kutta methods and a particular case of the symplectic SPARK methods [12]. In [12] it is shown how the symplectic SPARK method can be derived variationally.

The approach in this work for constructing variational integrators of higher order for constrained systems follows [20] and is based on the constrained Galerkin methods in [17]. A short summary of some results presented here are already given in [26]. The construction starts with the approximation of the continuous curves of the configuration q and λ via different polynomials. The integral of the augmented Lagrangian, i.e., the Lagrangian augmented by the scalar product $g(q) \cdot \lambda$, is approximated via appropriate quadrature formulas. The splitting of the augmented Lagrangian in the two parts Lagrangian and scalar product $g(q) \cdot \lambda$ enables the use of different quadrature formulas for each part. This is in contrast to the constrained Galerkin methods in [17]. Conditions on the degrees of the polynomials, the polynomial control points and the quadrature formulas are formulated, to ensure the solvability of the higher order constrained discrete Euler-Lagrange equations and to allow for high accuracy and stiffly accurate integration. The discrete augmented Lagrangian serves as a generating function for the variational integrators, constructed in this work, just as for the symplectic SPARK integrators in [12]. But in contrast to [17] and [12], the degree of the polynomial q_d is not restricted to equal the number of quadrature nodes of the quadrature formula approximating the integral of the Lagrangian here. Furthermore, in [12] the SPARK integrator is applied to a system of index 2 overdetermined DAEs. In this work, the preservation properties, such as symplecticity, preservation of momentum maps and the time reversibility of the constructed integrators are investigated analytically and

verified numerically. For the investigation of the time reversibility, a distinction between the discrete flow on configuration level only and on configuration and momentum level leads to different results. The order of convergence is determined numerically, revealing order reduction of the momentum and the Lagrange multiplier compared to the order of the configuration. A numerical analysis regarding accuracy versus efficiency shows that the presented integrators with high orders provide very accurate results together with low computational times.

Outline In Section 2, constrained Lagrangian dynamics and the discretization of the underlying variational principle, using linear polynomials for the approximation of the continuous curves, are recalled and the preservation properties are discussed. Section 3 deals with the construction of the constrained higher order variational integrators. The derivations base on the higher order variational integrators in [20] and extend them to the constrained case, see Section 3.1 and 3.2. In Section 3.3, conditions are formulated to reach linear independence of the higher order constrained discrete Euler-Lagrange equations and to obtain stiffly accurate integrators. In the following Sections 3.4.1 and 3.4.2, the preservation properties, such as symplecticity and preservation of momentum maps, are discussed. Furthermore, in Section 3.4.3 the time reversibility of the constructed integrators is investigated. A comparison with existing methods for index 3 DAEs in Section 3.5 embeds them into existing works and reveals the differences. In Section 4, the convergence order of the constructed integrators is investigated numerically and the preservation properties are demonstrated by numerical examples. A numerical analysis regarding the efficiency and accuracy is carried out for the most promising integrators. Finally, a conclusion is given in Section 5, together with an outlook on future work.

2 Variational mechanics for constrained systems

2.1 Constrained Lagrangian dynamics

This section presents a summary of the theoretical background following [17]. Consider an n-dimensional mechanical system defined on the configuration space Q being an n-dimensional vector space, e.g., $Q = \mathbb{R}^n$, with configuration vector $q(t) \in Q$ and velocity vector $\dot{q}(t) \in T_{q(t)}Q$, e.g., $\dot{q}(t) \in T_{q(t)}\mathbb{R}^n (= \mathbb{R}^n)$. The variable t denotes the time in the interval $t \in [t_0, t_N]$. For a mechanical system the Lagrangian $L : TQ \to \mathbb{R}$ is the difference of the kinetic energy $T(q, \dot{q})$ and the potential $V(q)$. Let the motion be constrained by a vector valued function of holonomic scleronomic constraints $g(q) = 0 \in \mathbb{R}^m$. Assuming that $0 \in \mathbb{R}^m$ is a regular value of g, the motion is constrained to the $(n - m)$-dimensional submanifold $C = g^{-1}(0) = \{q \mid q \in Q, g(q) = 0\} \subset Q$. The map $i : C \to Q$ embeds the submanifold C in Q and the tangential lift Ti gives a way to embed the submanifold TC in TQ. Making use of the Lagrange multiplier theorem the holonomic constraints can be included by augmenting a given Lagrangian by the scalar product $-g(q) \cdot \lambda$, where $\lambda(t) \in \mathbb{R}^m$ is the Lagrange multiplier. The so called augmented Lagrangian $\bar{L} : TQ \times \mathbb{R}^m \to \mathbb{R}$ is defined by

$$\bar{L}(q, \dot{q}, \lambda) = L(q, \dot{q}) - g(q) \cdot \lambda \tag{1}$$

The augmented action $\bar{S} : \mathcal{C}(Q \times \mathbb{R}^m) \to \mathbb{R}$ is the time integral of the augmented Lagrangian, i.e.,

$$\bar{S}(q, \lambda) = \int_{t_0}^{t_N} [L(q, \dot{q}) - g(q) \cdot \lambda] \, dt \tag{2}$$

with $\mathcal{C}(Q) = \mathcal{C}([t_0, t_N], Q; q_0, q_N)$ being the space of smooth functions $q : [t_0, t_N] \to Q$ satisfying $q(0) = q_0$ and $q(t_N) = q_N$, where q_0, $q_N \in C \subset Q$ are fixed endpoints, and $\mathcal{C}(\mathbb{R}^m) = \mathcal{C}([t_0, t_N], \mathbb{R}^m)$ being the space of curves $\lambda : [t_0, t_N] \to \mathbb{R}^m$ with no boundary conditions. Hamilton's principle seeks the curves $(q, \lambda) \in \mathcal{C}(Q \times \mathbb{R}^m)$ that extremize the augmented action. The demand of stationarity yields the constrained Euler-Lagrange equations

$$\begin{aligned} \frac{\partial L(q, \dot{q})}{\partial q} - \frac{d}{dt}\left(\frac{\partial L(q, \dot{q})}{\partial \dot{q}}\right) - G^T(q) \cdot \lambda = 0 \\ g(q) = 0 \end{aligned} \tag{3}$$

whereby $G(q) = Dg(q)$ denotes the $m \times n$ Jacobian of the constraints and is supposed to be of full row rank m. The term $-G^T(q) \cdot \lambda$ represents the constraint forces that prevent the system from deviation of the constraint submanifold C. The constrained Euler-Lagrange equations are index 3 DAEs of second order.

We assume that the Lagrangian L is hyperregular, such that the constrained Lagrangian flow $F_L : TQ|_C \to TQ|_C$ is well defined and the Legendre transform $\mathbb{F}L : TQ|_C \to T^*Q|_C$, with $\mathbb{F}L : (q, \dot{q}) \mapsto (q, \frac{\partial L}{\partial \dot{q}}) = (q, p)$ and p being the conjugate momentum, is a global diffeomorphism, where $TQ|_C$ respectively $T^*Q|_C$ contains all elements of the tangential space TQ respectively cotangential space T^*Q with basis points in C. The Hamiltonian H defined by $H(q, p) = \mathbb{F}L(q, \dot{q}) \cdot \dot{q} - L(q, \dot{q})$ is then hyperregular as well with Legendre transform $\mathbb{F}H = (\mathbb{F}L)^{-1} : T^*Q|_C \to TQ|_C$. Define $L^C = L|_{TC}$ as the restriction of L to the submanifold TC, such that $L^C = L \circ Ti$. This implies that L^C is regular when L is and the diagram on the left side in Fig. 1 commutes, with the projection $T^*i : T^*Q|_C \to T^*C$. As

Fig. 1 Relation between Lagrangian and Hamiltonian representations, the embeddings $Ti : TC \to TQ$, $\eta : T^*C \to T^*Q|_C$ and the projection $T^*i : T^*Q|_C \to T^*C$

the Lagrangian and Hamiltonian representations are equivalent, the embedding $\eta : T^*C \to T^*Q$ can be defined by requiring that the right diagram in Fig. 1 commutes, it reads

$$\eta(T^*C) = \{(q, p) \in T^*Q \mid g(q) = 0 \text{ and } G \cdot \frac{\partial H}{\partial p}(q, p) = 0\}$$

The term $G \cdot \frac{\partial H}{\partial p}(q, p)$ is obtained by differentiating the constraints $g(q)$ w.r.t. the time t with $\dot{q} = \frac{\partial H}{\partial p}(q, p)$ and is called hidden constraints. A projection map

$\mathbb{P} : T^*Q|_C \to \eta(T^*C)$ can be defined by $\mathbb{P} = \eta \circ T^*i$, reading in coordinates

$$\mathbb{P} = I - G^T(q) \left[G(q) \frac{\partial^2 H(q,p)}{\partial p^2} G^T(q) \right]^{-1} G(q) \frac{\partial^2 H(q,p)}{\partial p^2} \tag{4}$$

with I being the $n \times n$ identity matrix, [8], [14], [17]. While the dual T_q^*C consists of equivalence classes $[p]$ with $p' \in [p]$ iff $\langle p - p', \dot{q} \rangle = 0$ for all $\dot{q} \in T_qC$ with $\langle \cdot, \cdot \rangle$ being the canonical pairing, the projection to the embedding corresponds to the selection of a representative fulfilling the hidden constraints. Next, the preservation properties being characteristic for the dynamical system in (3) are discussed briefly.

Symmetry, symplecticity and energy behaviour The systems, considered here, are conservative. Thus, the total energy of the system is conserved along the solution of the Euler-Lagrange equations (3) and the Lagrangian flow is symmetric[1] and symplectic. The symplecticity of the Lagrangian flow of a conservative system is shown, e.g., in [17], both for unconstrained and for constrained systems.

Noether theorem The Noether theorem provides first integrals of the Euler-Lagrange equations. They are also called momentum maps. Let $L(q, \dot{q})$ be a regular Lagrangian of a dynamical system, constrained by holonomic constraints $g(q)$. If there is a one-parameter group of transformations $\Phi = \{\phi_u : u \in \mathbb{R}\}$, leaving the Lagrangian invariant, i.e., $L(\phi_u(q), \phi_u'(q)\dot{q}) = L(q, \dot{q})$, $\forall (q, \dot{q}) \in TQ, \forall u \in \mathbb{R}$, and the constraints $g(\phi_u(q)) = 0, \forall q \in C, \forall u \in \mathbb{R}$ satisfied, then a first integral of the Euler-Lagrange equations can be defined by

$$I(q,p) = p^T a(q) \tag{5}$$

whereby $a(q) = \frac{d}{du}\phi_u(q)|_{u=0}$ is a vector field with flow $\phi_u(q)$ and p is the conjugate momentum defined by the Legendre transform $p = \frac{\partial L}{\partial \dot{q}}$.

A proof of the Noether theorem for unconstrained systems can be found in [5]. The proof can be extended to systems with holonomic constraints, given that $g(\phi_u(q)) = 0$ holds $\forall q \in C$.

In [17] the validity of the Noether theorem in the constrained case is shown via the relation of the unconstrained system with the standard Lagrangian $L : TQ \to \mathbb{R}$ and the constrained system with the restricted Lagrangian $L^C = L_{|TC} : TC \to \mathbb{R}$ defined by $L^C = L \circ Ti$.

2.2 Constrained discrete variational dynamics

The main idea of variational integrators is based on the discretization of the variational principle instead of solving the resulting equations of motion.
The path $q : [t_0, t_N] \to Q$ is replaced by a discrete path $\{q_k\}_{k=0}^N : \{t_k\}_{k=0}^N = \{t_0, t_0 + h, \ldots, t_0 + kh, \ldots, t_0 + Nh = t_N\} \to Q$. Let the time step h be constant. The configuration q_k holds as an approximation to $q(t_k)$. Similarly the Lagrange multipliers are approximated by defining λ_k as the approximation to $\lambda(t_k)$, with $\{\lambda_k\}_{k=0}^N : \{t_k\}_{k=0}^N \to \mathbb{R}^m$. The curves q and λ between two neighbouring time

[1] As in [5] (Ch. V, Def. 1.4), symmetry and time reversibility are used synonymously here, a definition is given in Section 3.4.3

points t_k and t_{k+1} are approximated via the polynomials q_d respectively λ_d. Linear polynomials for both are considered first. The approximate integral in $[t_k, t_{k+1}]$ of the augmented action $\bar{S}$ in (2) is called the discrete augmented Lagrangian $\bar{L}_d : Q \times Q \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$

$$\bar{L}_d(q_k, q_{k+1}, \lambda_k, \lambda_{k+1}) \approx \int_{t_k}^{t_{k+1}} [L(q, \dot{q}) - g(q) \cdot \lambda] \, dt \tag{6}$$

$$L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q, \dot{q}) \, dt \tag{7}$$

$$g_d(q_k, q_{k+1}, \lambda_k, \lambda_{k+1}) \approx \int_{t_k}^{t_{k+1}} g(q) \cdot \lambda \, dt \tag{8}$$

In (7), L_d approximates the integral in $[t_k, t_{k+1}]$ of the Lagrangian L (briefly named the Lagrangian integral) and in (8), g_d approximates the integral in $[t_k, t_{k+1}]$ of the scalar product of the constraints and the Lagrange multipliers (briefly named constraints integral). For the entire time interval $[t_0, t_N]$ the approximation of the augmented action is the discrete augmented action sum

$$\bar{S}_d = \sum_{k=0}^{N-1} \bar{L}_d(q_k, q_{k+1}, \lambda_k, \lambda_{k+1}) \tag{9}$$

The variation of the discrete augmented action sum (9) w.r.t. $\{\delta q_k\}_{k=1}^{N-1} \forall \delta q_k \in T_{q_k} Q$, $\delta q_0 = \delta q_N = 0$, and w.r.t. $\{\delta \lambda_k\}_{k=0}^{N} \forall \delta \lambda_k \in \mathbb{R}^m$ and requiring its stationarity gives the constrained discrete Euler-Lagrange equations. The quadrature formulas for L_d and g_d determine the integrator. In particular, when approximating the constraints integral via the Lobatto quadrature of order two

$$g_d = \frac{h}{2}(g(q_k) \cdot \lambda_k + g(q_{k+1}) \cdot \lambda_{k+1})$$

whereas for the approximation of the Lagrangian integral various quadrature formulas can be used (e.g., the midpoint approximation, Gauss quadrature or also the Lobatto quadrature), the constrained discrete Euler-Lagrange equations read

$$\begin{aligned} D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) - G_d^T(q_k) \cdot \lambda_k &= 0 \\ g(q_{k+1}) &= 0 \end{aligned} \tag{10}$$

with $hG^T = G_d^T$ and $D_\alpha L_d$ being the partial derivative of the discrete Lagrangian w.r.t. the α-th argument. The system's evolution on momentum level can be obtained from the constrained discrete Legendre transform $\mathbb{F}^{\pm}_{\bar{L}_d} : Q \times Q|_{q_k \in C} \to T^*Q|_C$

$$\mathbb{F}^+_{\bar{L}_d} : (q_{k-1}, q_k) \mapsto (q_k, p_k^+) = \left(q_k, D_2 L_d(q_{k-1}, q_k) - \frac{1}{2} G_d^T(q_k) \cdot \lambda_k \right)$$

$$\mathbb{F}^-_{\bar{L}_d} : (q_k, q_{k+1}) \mapsto (q_k, p_k^-) = \left(q_k, -D_1 L_d(q_k, q_{k+1}) + \frac{1}{2} G_d^T(q_k) \cdot \lambda_k \right)$$

Note that (10) can be interpreted as enforcing the matching of momenta $p_k^+ - p_k^- = 0$. Thus, there is a unique momentum p_k at each time node t_k along the discrete trajectory, which not necessarily fulfills the hidden constraints. The solution of

(10) together with the discrete Legendre transform yields the discrete Hamiltonian map $\tilde{F}_{\bar{L}_d} : T^*Q|_C \to T^*Q|_C$ with $\tilde{F}_{\bar{L}_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$. When using the Lobatto quadrature of order two for the approximation of the Lagrangian integral with L of the form $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$ and M being the mass matrix, (10) results in the SHAKE algorithm [17]. As SHAKE is a famous representative of the variational integrator, it is discussed widely and its main properties are summarized here briefly.

Symmetry, symplecticity and energy behaviour In the literature the properties of SHAKE are not described consistently. In [13] the SHAKE algorithm is declared to be time reversible. It is proved that SHAKE preserves the wedge product $dq_{k+1} \wedge dp_{k+1} = dq_k \wedge dp_k$, "[...]although SHAKE is not, strictly speaking, a symplectic method, as the meshpoint velocities are not tangent to the constraint manifold[...]", because the hidden constraints, here $G(q_k) \cdot M^{-1} \cdot p_k = 0$, typically fail to be satisfied. In [18], the SHAKE algorithm for Hamiltonian systems with cosiotropic constraints is investigated geometrically. An index 3 DAE, as in (3), describes a special case of this class of constrained systems. It is shown, that the numerical solution of SHAKE fulfills the configuration constraints but not the hidden constraints. They prove that the SHAKE map preserves the wedge product and say that it is thus symplectic. In [18], SHAKE is negated to be symmetric. In [17], SHAKE is described as a method that conserves the symplectic structure. The reason for different statements concerning the time reversibility of SHAKE is discussed in the remark after Theorem 2.

In accordance with the general theory of symplectic integrators, the variational integrator (10) shows excellent energy properties. The energy does not grow or decrease in time due to numerical errors but stays bounded [21], [2]. This is interesting especially in case of long-time simulations.

Discrete Noether Theorem In the presence of symmetry in the discrete Lagrangian (7) where the corresponding transformation leaves the constraints manifold C invariant, the variational integrator (10) preserves discrete momentum maps [17].

3 Higher order variational integrators for constrained systems

3.1 Approximation of the augmented action integral

The following derivations are based on the higher order variational integrators in [20], and extend them to the constrained case. The approximation of the augmented action integral consists of two approximation steps. The first step is the approximation of the continuous curves q and λ on the time interval $[0, h]$. In contrast to the approach in Section 2.2, polynomials of higher degree instead of linear polynomials are used for the discretization. As a second step, the integral of the augmented Lagrangian is approximated by appropriate quadrature formulas.

The polynomial q_d of degree s approximates the continuous curve q on the time interval $[0, h]$, thus the space of trajectories $\mathcal{C}([0, h], Q) = \{q : [0, h] \to Q \mid q(0) = q_k^0, q(h) = q_{k+1}^0\}$ reduces to the the space of trajectories $\mathcal{C}^s([0, h], Q) \subset \mathcal{C}([0, h], Q)$ given by

$$\mathcal{C}^s([0, h], Q) = \{q \in \mathcal{C}([0, h], Q) \mid q \in \Pi^s\}$$

whereby Π^s is the space of polynomials of degree s. A polynomial of degree s is uniquely defined by $s+1$ configurations $q_k = (q_k^0, \ldots, q_k^s) \in Q^{s+1}$ at $s+1$ control points $0 = d_0 < d_1 < \ldots < d_{s-1} < d_s = 1$, such that the polynomial passes through each q_k^ν at the time $d_\nu h$, $\nu = 0, \ldots, s$. With the Lagrange polynomials $l_{\nu,s} : [0,h] \to \mathbb{R}$ the polynomial $q_d(t; q_k, h)$, $t \in [0,h]$, has the following form

$$q_d(t; q_k, h) = \sum_{\nu=0}^{s} q_k^\nu \, l_{\nu,s}\left(\frac{t}{h}\right) \qquad \text{with} \qquad l_{\nu,s}\left(\frac{t}{h}\right) = \prod_{0 \le j \le s, j \neq \nu} \frac{\frac{t}{h} - d_j}{d_\nu - d_j} \quad (11)$$

It can be checked easily, that $q_d(d_j h; q_k, h) = q_k^j$ is true for all $j = 0, \ldots, s$ with

$$l_{\nu,s}(d_j) = \begin{cases} 1 & , j = \nu \\ 0 & , j \neq \nu \end{cases}$$

Differentiating q_d w.r.t. t, an approximation of $\dot{q}$ on $[0,h]$ is obtained

$$\dot{q}_d(t; q_k, h) = \frac{1}{h} \sum_{\nu=0}^{s} q_k^\nu \, \dot{l}_{\nu,s}\left(\frac{t}{h}\right)$$

Let the time interval $[t_0, t_N]$, with $t_0 = 0$, be divided in $N = t_N/h$ subintervals of lengths h such that

$$[t_0, t_N] = \bigcup_{k=0}^{N-1} [kh, (k+1)h]$$

On each subinterval, the continuous curve q is approximated by a polynomial $q_{d,k} : [kh, (k+1)h] \to Q$, $k = 0, \ldots, N-1$. To get a continuous approximation of the trajectory q on $[t_0, t_N]$, the conditions $q_{k-1}^s = q_k^0$, $k = 1, \ldots, N-1$ must be fulfilled.

A similar procedure is applied to discretize λ. The space of trajectories $\mathcal{C}([0,h], \mathbb{R}^m)$ reduces to $\mathcal{C}^w([0,h], \mathbb{R}^m) = \{\lambda \in \mathcal{C}([0,h], \mathbb{R}^m) \mid \lambda \in \Pi^w\}$. Given $w+1$ control points $\widetilde{d}_0 = 0 < \widetilde{d}_1 < \ldots < \widetilde{d}_{w-1} < \widetilde{d}_w = 1$ and $w+1$ Lagrange-multipliers $\lambda_k = (\lambda_k^0, \ldots, \lambda_k^w) \in (\mathbb{R}^m)^{w+1}$, the polynomial $\lambda_d(t; \lambda_k, h)$, $t \in [0,h]$ is uniquely defined by (12). Note that the control points $\tilde{d}_j$, $j = 0, \ldots, w$ do not have to match the control points d_j, $j = 0, \ldots, s$, neither has the degree w of the polynomial λ_d to equal the degree s of q_d.

$$\lambda_d(t; \lambda_k, h) = \sum_{\mu=0}^{w} \lambda_k^\mu \, \widetilde{l}_{\mu,w}\left(\frac{t}{h}\right) \qquad \widetilde{l}_{\mu,w}\left(\frac{t}{h}\right) = \prod_{0 \le j \le w, j \neq \mu} \frac{\frac{t}{h} - \widetilde{d}_j}{\widetilde{d}_\mu - \widetilde{d}_j} \quad (12)$$

To get a continuous approximation of λ on $[t_0, t_N]$, the conditions $\lambda_{k-1}^w = \lambda_k^0$, $k = 1, \ldots, N-1$ must hold.

For the approximation of the augmented action integral $\bar{S}$ in (2) on each time subinterval $[kh, (k+1)h]$, $k = 0, \ldots, N-1$ different quadrature formulas for the two integrals, the Lagrangian integral and the constraints integral, are considered. The quadrature rule $(b_i, c_i)_{i=1}^r$ is chosen for the Lagrangian integral and $(e_i, f_i)_{i=1}^z$ for the constraints integral. The quadrature rules are w.r.t. the time $[0,1]$ with quadrature nodes c_i respectively f_i and the associated weights b_i respectively e_i.

The curves q, $\dot{q}$ and λ are replaced by the piecewise polynomials q_d, $\dot{q}_d$ and λ_d such that the discrete augmented Lagrangian $\bar{L}_d : Q^{s+1} \times (\mathbb{R}^m)^{w+1} \times \mathbb{R} \to \mathbb{R}$ reads

$$\begin{aligned}
\bar{L}_d(q_k, \lambda_k, h) &= L_d(q_k, h) - g_d(q_k, \lambda_k, h) \approx \int_{kh}^{(k+1)h} [L(q, \dot{q}) - g(q) \cdot \lambda] \, dt \\
\bar{L}_d(q_k, \lambda_k, h) &= h \sum_{i=1}^{r} b_i L(q_d(c_i h; q_k, h), \dot{q}_d(c_i h; q_k, h)) \\
&\quad - h \sum_{i=1}^{z} e_i \left[g(q_d(f_i h; q_k, h)) \cdot \lambda_d(f_i h; \lambda_k, h) \right] \qquad (13)
\end{aligned}$$

In the following the abbreviations $\bar{L}_d(q_k, \lambda_k)$, $q_d(t; q_k)$ and $\lambda_d(t; \lambda_k)$ will be used instead of $\bar{L}_d(q_k, \lambda_k, h)$, $q_d(t; q_k, h)$ and $\lambda_d(t; \lambda_k, h)$. Finally the approximation of the augmented action integral $\bar{S}$ in (2) on the entire time interval $[t_0, t_N]$ can be written as

$$\bar{S}_d(q_0, \ldots, q_{N-1}, \lambda_0, \ldots, \lambda_{N-1}) = \sum_{k=0}^{N-1} \bar{L}_d(q_k, \lambda_k) \qquad (14)$$

3.2 Discrete Hamilton's principle for constrained systems

Regarding to Hamilton's principle, the discrete augmented action sum $\bar{S}_d$ in (14) has to be stationary. To find the discrete curves extremizing the discrete augmented action sum $\bar{S}_d$, the derivatives of $\bar{S}_d$ w.r.t. q_k^ν and λ_k^μ have to vanish $\forall\ k = 0, \ldots, N-1$, $\nu = 0, \ldots, s$, $\mu = 0, \ldots, w$. The variations of the endpoints $q(t_0) = q_0^0$, $q(t_N) = q_N^0 \in C \times C$ are zero, $\delta q_0^0 = \delta q_N^0 = 0$. Thus, the constrained discrete Euler-Lagrange equations are obtained

$$\begin{aligned}
0 =& p_0^0 + D_1 \bar{L}_d(q_0^0, \ldots, q_0^s, \lambda_0^0, \ldots, \lambda_0^w) \\
0 =& D_\alpha \bar{L}_d(q_k^0, \ldots, q_k^s, \lambda_k^0, \ldots, \lambda_k^w) \quad \alpha = 2, \ldots, s && k = 0, \ldots, N-1 \\
0 =& D_{s+1} \bar{L}_d(q_k^0, \ldots, q_k^s, \lambda_k^0, \ldots, \lambda_k^w) \\
&+ D_1 \bar{L}_d(q_{k+1}^0, \ldots, q_{k+1}^s, \lambda_{k+1}^0, \ldots, \lambda_{k+1}^w) && k = 0, \ldots, N-2 \\
0 =& D_{s+2} \bar{L}_d(q_0^0, \ldots, q_0^s, \lambda_0^0, \ldots, \lambda_0^w) && (15) \\
0 =& D_{s+1+\alpha} \bar{L}_d(q_k^0, \ldots, q_k^s, \lambda_k^0, \ldots, \lambda_k^w) \quad \alpha = 2, \ldots, w && k = 0, \ldots, N-1 \\
0 =& D_{s+w+2} \bar{L}_d(q_k^0, \ldots, q_k^s, \lambda_k^0, \ldots, \lambda_k^w) \\
&+ D_{s+2} \bar{L}(q_{k+1}^0, \ldots, q_{k+1}^s, \lambda_{k+1}^0, \ldots, \lambda_{k+1}^w) && k = 0, \ldots, N-2 \\
0 =& D_{s+w+2} \bar{L}_d(q_{N-1}^0, \ldots, q_{N-1}^s, \lambda_{N-1}^0, \ldots, \lambda_{N-1}^w)
\end{aligned}$$

with the first equation being the constrained discrete Legendre transform $\mathbb{F}^-_{\bar{L}_d} : (q_0^0, q_1^0) \mapsto (q_0^0, p_0^0)$. In (15) the configuration q_0^0 and the momentum p_0^0 at time point $t_0 = 0$ are assumed as given and q_N^0 as unknown. The definitions of the constrained discrete Legendre transforms $\mathbb{F}^\pm_{\bar{L}_d} : Q \times Q|_{q_k^0 \in C} \to T^*Q|_C$ read as follows

$$\mathbb{F}^+_{\bar{L}_d} : (q_{k-1}^0, q_{k-1}^s) \mapsto (q_{k-1}^s, p_{k-1}^{s^+}) = (q_{k-1}^s, D_{s+1} \bar{L}_d(q_{k-1}, \lambda_{k-1})) \qquad (16)$$

$$\mathbb{F}^-_{\bar{L}_d} : (q_k^0, q_k^s) \mapsto (q_k^0, p_k^{0^-}) = (q_k^0, -D_1 \bar{L}_d(q_k, \lambda_k)) \qquad (17)$$

One recognizes the constrained discrete Euler-Lagrange equations in $p_{k-1}^{s^+} - p_k^{0^-} = 0$, such that along the solution of (15) the momentum $p_k^0 = p_{k-1}^{s^+} = p_k^{0^-}$ is unique. However, p_k^0 does not necessarily fulfill the hidden constraints.

3.3 Construction of the constrained higher order variational integrators

The polynomial q_d in (11) and λ_d in (12) and the quadrature formulas in (13) can not be used in arbitrary combinations for the approximation of the augmented action. For example, consider a dynamical system with given initial conditions q_0^0 and p_0^0 at time point $t_0 = 0$. For the first time interval $[0, h]$, the augmented discrete Lagrangian (13) reads $\bar{L}_d(q_0, \lambda_0) = \bar{L}_d(q_0^0, \ldots, q_0^s,\ \lambda_0^0, \ldots, \lambda_0^w)$ and depends on $(s + w + 1)$ unknowns, as the Lagrange-multiplier λ_0^0 is assumed to be unknown. Considering (15) one can see that there are only $(s + w)$ equations to determine the configurations $q_0^1, \ldots, q_0^s$ and the Lagrange-multipliers $\lambda_0^0, \ldots, \lambda_0^w$. These are the Legendre transform and the equations obtained by differentiating $\bar{L}_d(q_0, \lambda_0)$ w.r.t. $q_0^1, \ldots, q_0^{s-1}$ and $\lambda_0^0, \ldots, \lambda_0^{w-1}$. Note, that the variations w.r.t. q_0^s and λ_0^w bring in new unknowns. Furthermore, when dealing with index 3 DAEs, so called stiffly accurate Runge-Kutta methods provide highly accurate results [4], [9], [10], [3], [8]. The stiffly accurate condition implies that $q_1 = Q_s$, whereby Q_s is the internal stage at time node c_s of the Runge-Kutta method.

Remark on stiffly accurate Stiffly accurate integration scheme means here that the configurations q_k^0 at the time nodes t_k fulfill the constraints, i.e., $q_k^0 \in C$, $k = 0, \ldots, N$.

In the following, we give conditions that ensure the solvability of the discrete Euler-Lagrange equations and an additional condition for a stiffly accurate integration scheme.

Assumption 1 The Lagrangian L is regular and the order of the quadrature formula $(b_i, c_i)_{i=1}^r$ for approximating the Lagrangian integral is high enough such that the discrete Lagrangian flow is well defined [6].

Theorem 1 *Under assumption* 1*, the following conditions*

1. *All quadrature nodes f_i, $i = 1, \ldots, z$ are part of the control points $\tilde{d}_j$, $j = 0, \ldots, w$ of the polynomial λ_d.*
2. *The degree s of the polynomial q_d is greater or equal to the degree w of the polynomial λ_d, i.e., $s \geq w$ if the constraints integral is approximated via the Lobatto quadrature.*
   The degree s of the polynomial q_d is greater or equal to $w - 1$, i.e., $s \geq w - 1$ if the constraints integral is approximated via the Gauss quadrature.

are sufficient to ensure that the discrete Euler-Lagrange equations are solvable. If additionally the following condition holds

3. *The quadrature node f_z equals one, i.e., $f_z = 1$.*

the integration scheme is stiffly accurate.

Proof. Condition 1 causes the number of unknowns to equal the number of equations in one time step. When condition 1 holds, condition 2 ensures the linear independence of the equations. Thus, condition 1 together with condition 2 assure

the solvability of the discrete Euler-Lagrange equations. A stiffly accurate integration scheme is reached by condition 1 together with condition 3. The conditions given in Theorem 1 are discussed now in detail.

Condition 1 Let condition 1 hold. With the control points $\tilde{d}_j$, $j = 0, \ldots, w$ of the polynomial λ_d matching the quadrature nodes f_i, $i = 1, \ldots, z$, the number of equations equals the number of unknowns in one time step. Note, that the quadrature nodes f_i, $i = 1, \ldots, z$ are used for the approximation of g_d in (13) and the boundary control points $\tilde{d}_0 = 0$ and $\tilde{d}_w = 1$ of the polynomial λ_d are fixed.

In this work, the quadrature formulas Lobatto and Gauss are used. In the following the calculation of g_d in (13) via the Lobatto or via the Gauss quadrature is considered separately, whereas the approximation of the Lagrangian integral is not specified further, see Assumption 1.

In the first case, when approximating the constraints integral via the Lobatto quadrature $(e_i, f_i)_{i=1}^{z}$, the control points of the polynomial λ_d are

$$0 = \tilde{d}_0 = f_1, \tilde{d}_1 = f_2, \ldots, \tilde{d}_w = f_z = 1 \qquad \text{with} \quad z = w + 1$$

As a consequence, no linear combinations of λ_d occur in the approximation of the constraints integral because the evaluation of λ_d at a quadrature node f_{i+1} being equal to the control point $\tilde{d}_i$ yields only the corresponding Lagrange-multiplier λ_k^i, i.e.,

$$\lambda_d(f_{i+1}h; \lambda_k) = \lambda_d(\tilde{d}_i h; \lambda_k) = \lambda_k^i, \qquad i = 0, \ldots, w$$

The resulting augmented discrete Lagrangian reads

$$\bar{L}_d(q_k, \lambda_k) = L_d(q_k) - g_d(q_k, \lambda_k) \tag{18}$$

with

$$L_d(q_k) = h \sum_{i=1}^{r} b_i L(q_d(c_i h; q_k), \dot{q}_d(c_i h; q_k)) \tag{19}$$

$$g_d(q_k, \lambda_k) = h \sum_{i=0}^{w} e_{i+1} \left[g(q_d(\tilde{d}_i h; q_k)) \cdot \lambda_k^i \right] \tag{20}$$

Note that the variation of $\bar{L}_d(q_0, \lambda_0)$ w.r.t. λ_0^0 now yields $he_1 g(q_0^0) = 0$ which is automatically satisfied since q_0^0 is assumed to be consistent. The variation w.r.t. $\lambda_0^w = \lambda_1^0$ yields

$$\begin{aligned} 0 &= D_{s+w+2}\bar{L}_d(q_0^0, \ldots, q_0^s, \lambda_0^0, \ldots, \lambda_0^w) + D_{s+2}\bar{L}_d(q_1^0, \ldots, q_1^s, \lambda_1^0, \ldots, \lambda_1^w) \\ &= -he_{w+1}g(q_0^s) - he_1 g(q_1^0) = -2he_1 g(q_0^s) = -2he_1 g(q_1^0) \end{aligned} \tag{21}$$

taking account of the symmetry of the weights of the Lobatto quadrature $e_{i+1} = e_{z-i}$, $i = 0, \ldots, z-1$. Equation (21) can be used to determine the unknowns in the first time interval. With condition 1 and the Lobatto quadrature for calculating

g_d, the constrained discrete Euler-Lagrange equations for the entire time interval $[t_0, t_N]$ read

$$
\begin{aligned}
0 =& p_0^0 + D_1 \bar{L}_d(q_0, \lambda_0) \\
=& p_0^0 + D_1 L_d(q_0) - h e_1 G^T(q_0^0) \cdot \lambda_0^0 + h \sum_{i=1}^{w-1} e_{i+1} G^T(q_d(\tilde{d}_i h; q_0)) l_{0,s}(\tilde{d}_i) \cdot \lambda_0^i \\
0 =& D_\nu \bar{L}_d(q_k, \lambda_k) = D_\nu L_d(q_k) - h \sum_{i=1}^{w-1} e_{i+1} G^T(q_d(\tilde{d}_i h; q_k)) l_{\nu-1,s}(\tilde{d}_i) \cdot \lambda_k^i \\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \nu = 2, \dots, s \quad k = 0, \dots, N-1 \\
0 =& D_{s+1} \bar{L}_d(q_k, \lambda_k) + D_1 \bar{L}_d(q_{k+1}, \lambda_{k+1}) = \qquad\qquad (22) \\
& D_{s+1} L_d(q_k) - h \sum_{i=1}^{w} e_{i+1} G^T(q_d(\tilde{d}_i h; q_k)) l_{s,s}(\tilde{d}_i) \cdot \lambda_k^i + \\
& D_1 L_d(q_{k+1}) - h \sum_{i=0}^{w-1} e_{i+1} G^T(q_d(\tilde{d}_i h; q_{k+1})) l_{0,s}(\tilde{d}_i) \cdot \lambda_{k+1}^i \qquad k = 0, \dots, N-2 \\
0 =& g(q_d(\tilde{d}_i h; q_k)) \qquad\qquad\qquad\qquad i = 1, \dots, w-1 \qquad k = 0, \dots, N-1 \\
0 =& g(q_d(\tilde{d}_w h; q_k)) = g(q_k^s) \qquad\qquad\qquad\qquad\qquad\quad k = 0, \dots, N-1
\end{aligned}
$$

with the first equation being the constrained discrete Legendre transform $\mathbb{F}^-_{\bar{L}_d} : (q_0^0, q_1^0) \mapsto (q_0^0, p_0^0)$. The Lagrange-multiplier λ_N^w does not appear in the set of equations anymore. Regarding the equations for one time step, assume $q_{k-1} = (q_{k-1}^0, \dots, q_{k-1}^s)$ and $\lambda_{k-1}^0, \dots, \lambda_{k-1}^{w-1}$ as given, respectively p_0^0 and q_0^0 in the first time step, then the number of equations in (22) matches the number of unknown variables $q_k^1, \dots, q_k^s$ and $\lambda_k^0, \dots, \lambda_k^{w-1}$.

In the second case, the Gauss quadrature is used to approximate the constraints integral and thus, if condition 1 holds, the control points of the polynomial λ_d are as follows

$$\tilde{d}_1 = f_1, \tilde{d}_2 = f_2, \dots, \tilde{d}_{w-1} = f_z \qquad \text{with} \quad z = w - 1 \tag{23}$$

The boundaries of the time interval are not used in the Gauss quadrature and consequently the number of the polynomial control points $w + 1$ is larger by two than the number of quadrature nodes z, with $\tilde{d}_0 = 0$ and $\tilde{d}_w = 1$. The augmented discrete Lagrangian $\bar{L}_d$ is composed by (19) and

$$g_d(q_k, \lambda_k) = h \sum_{i=1}^{w-1} e_i \left[g(q_d(\tilde{d}_i h; q_k)) \cdot \lambda_k^i \right] \tag{24}$$

In (24), the Lagrange multipliers λ_k^0 and λ_k^w do not appear and consequently neither in the corresponding discrete Euler-Lagrange equations. For given configurations $q_{k-1} = (q_{k-1}^0, \dots, q_{k-1}^s)$ and Lagrange multipliers $\lambda_{k-1}^1, \dots, \lambda_{k-1}^{w-1}$, the number of unknowns $q_k^1, \dots, q_k^s$ and $\lambda_k^1, \dots, \lambda_k^{w-1}$ is equal to the number of the corresponding discrete Euler-Lagrange equations.

Condition 2 When condition 1 holds, condition 2 ensures the linear independence of the discrete Euler-Lagrange equations in one time interval. The following discussion starts from a general point of view, without the assumption that condition 1 or 2 holds. The derivatives of the discrete augmented Lagrangian w.r.t. the Lagrange multipliers λ_k^μ, $\mu = 0, \dots, w-1$, see (15), read

$$\begin{aligned}
&\sum_{i=1}^{z} \left(\tilde{l}_{0,w}(f_i)\right) e_i g(q_d(f_i h; q_k)) = \sum_{i=1}^{z} \left(\tilde{l}_{w,w}(f_i)\right) e_i g(q_d(f_i h; q_{k-1})) \\
&\sum_{i=1}^{z} \left(\tilde{l}_{\mu,w}(f_i)\right) e_i g(q_d(f_i h; q_k)) = 0 \qquad \mu = 1, \dots w-1
\end{aligned} \tag{25}$$

Linear dependence between the equations in (25) can occur. To get insight, the rank of the Jacobian of (25) is investigated,

$$\begin{aligned}
\frac{\partial \bar{L}}{\partial q_k^\nu \partial \lambda_k^\mu} &= \tilde{L}\tilde{G} \\
\text{with } \{\tilde{L}\}_{\mu,i} &= \tilde{l}_{\mu,w}(f_i) && \mu = 0, \dots, w-1, \quad i = 1, \dots, z \\
\{\tilde{G}\}_{i,\nu} &= e_i G(q_d(f_i h)) l_{\nu,s}(f_i) && i = 1, \dots, z, \quad \nu = 1, \dots, s
\end{aligned}$$

The rank of the single matrices are $\mathrm{rk}(\tilde{L}) = \min(\tilde{w}, \tilde{z})$ and $\mathrm{rk}(\tilde{G}) = \min(\tilde{z}, s)$, whereas $\tilde{w}$ and $\tilde{z}$ depend on the used quadrature formula. For example, when g_d in (13) is calculated via the Lobatto quadrature, it holds $\tilde{w} = w$ and $\tilde{z} = z - 2$. This is because $g(q_d(f_1)) = g(q_k^0)$ derived w.r.t. $q_k^1, \dots, q_k^s$ yields the zero vector and $\tilde{l}_{\mu,w}(f_z) = 0$, $\mu = 0, \dots, w-1$, such that the z-th column of $\tilde{L}$ is also the zero vector. The rank of the matrix multiplication $\tilde{L}\tilde{G}$ fulfills the following inequality, where the lower bound origins from Sylvester's rank inequality

$$\mathrm{rk}(\tilde{L}) + \mathrm{rk}(\tilde{G}) - \tilde{z} \leq \mathrm{rk}(\tilde{L}\tilde{G}) \leq \min(\tilde{w}, \tilde{z}, s)$$

Discussing all cases,

$$\mathrm{rk}(\tilde{L}\tilde{G}) = \min(\tilde{w}, \tilde{z}, s) \tag{26}$$

holds except for the case when $\tilde{z} > \tilde{w}$ and $\tilde{z} > s$ where the rank might be reduced $\mathrm{rk}(\tilde{L}\tilde{G}) \leq min(\tilde{w}, s)$. Let's assume condition 1 holds. Then this case can not occur, since then $\tilde{z} = \tilde{w}$. For the row rank of $\tilde{L}\tilde{G}$ to be full, it can be seen from (26) that condition 2 must hold. In particular, when the Gauss quadrature is used to calculate g_d, it holds $\tilde{w} = \tilde{z} = w - 1$. Consequently, there are $s + \min(w-1, w-1, s)$ linearly independent equations to determine the $s + w - 1$ unknowns $q_k^1, \dots, q_k^s, \lambda_k^1, \dots, \lambda_k^{w-1}$. Thus, $s \geq w - 1$ must hold. Using the Lobatto quadrature yields $\tilde{w} = \tilde{z} = w$. Thus, the linear independence of the equations (22) is given, if $s \geq w$. This ensures that the number of linearly independent equations, i.e., $s + \min(w, w, s)$, equals the number of the $(s + w)$ unknowns $q_k^1, \dots, q_k^s, \lambda_k^0, \dots, \lambda_k^{w-1}$. Note, when condition 1 holds, the differentiation of $\bar{L}_d$ w.r.t. the Lagrange-multipliers yields only the second equation in (25) with $\mu = 1, \dots, w$ when the Lobatto quadrature is used for calculating g_d. Condition 1 and 2 together cause $\tilde{L}$ to be of full rank and as the right hand side is zero, the equations simplify to $g(q_d(f_i h; q_k)) = 0$, $i = 1, \dots, w-1$ (Gauss) respectively $i = 2, \dots, w+1$ (Lobatto).

Condition 3 If condition 1 and condition 3 are fulfilled, the integration scheme is stiffly accurate. Let only condition 3 be fulfilled. The variation of $\bar{L}_d$ w.r.t. to the Lagrange multipliers yields the discrete constraints. As the Lagrange multipliers only occur in the constraints integral, the consideration of g_d suffices here. The approximation of the constraints integral in (13) reads

$$g_d = h \sum_{i=1}^{z-1} e_i \left[g(q_d(f_i h; q_k)) \cdot \lambda_d(f_i h; \lambda_k) \right] + h e_z \left[g(q_k^s) \cdot \lambda_k^w \right] \tag{27}$$

where condition 3, i.e., $f_z = 1$, causes the last term in (27) with $q_d(f_z h; q_k) = q_d(h; q_k) = q_k^s$ and $\lambda_d(f_z h; \lambda_k) = \lambda_d(h; \lambda_k) = \lambda_k^w$. Let in addition condition 1 hold. Then, the variation of g_d in (27) w.r.t. λ_k^w yields

$$0 = h e_z g(q_k^s) \qquad \text{if } f_1 \neq 0 \tag{28}$$

$$0 = h e_z g(q_k^s) + h e_1 g(q_{k+1}^0) = h(e_z + e_1) g(q_k^s) \qquad \text{if } f_1 = 0 \tag{29}$$

Both equations, (28) and (29), formulate the stiffly accurate condition. □

Remark on stiffly accurate condition Equation (29) can be found in (21) with $z = w+1$ and therefore also in the last equation in (22) with $\tilde{d}_w = f_z = 1$ where the integration scheme (22) bases on the calculation of g_d via the Lobatto quadrature when condition 1 holds. When the quadrature nodes of g_d and the control points of λ_d do not match (condition 1), the fulfillment of the stiffly accurate condition fails, even when the Lobatto quadrature rule is used. Then, the variation w.r.t. $\lambda_{k-1}^w = \lambda_k^0$ only yields a weighted sum of the constraints $g(q_d(f_i h; q_{k-1}))$ and $g(q_d(f_i h; q_k))$ evaluated at the quadrature nodes f_i, $i = 1, \ldots, z$ of g_d. Conversely, when condition 1 is fulfilled but condition 3 not, i.e., $f_z \neq 1$, the Lagrange multiplier λ_k^w does not occur in the approximation of the constraints integral and the last term in (27) is replaced by $h e_z \left[g(q_d(f_z h; q_k) \cdot \lambda_k^{w-1} \right]$, with $q_d(f_z h; q_k) \neq q_k^s$. Thus, the stiffly accurate condition lacks. As an example consider the Gauss quadrature for calculating g_d, see (24).

Due to condition 1, the degree w of the polynomial λ_d is coupled with the order of the quadrature formula $(f_i, e_i)_{i=1}^z$. To denote which quadrature formula of which order is used, some abbreviations are introduced. *ordL* denotes the order of the quadrature formula used to approximate the Lagrangian integral. *ordZ* denotes the order of the quadrature formula used to approximate the constraints integral. The name of the quadrature rule follows in brackets, whereby (Gau) means Gauss quadrature and (Lob) Lobatto quadrature. The correlation of the number of quadrature nodes n, here n can be r or z, and the order *ord* of the quadrature formula is given via $ord = 2n$ (Gau) and $ord = 2n - 2$ (Lob) (cf., e.g., [7], [22]). As seen before, the integrator is not stiffly accurate, when the Gauss quadrature is used for the approximation of the constraints integral. A numerical drift of the constraint manifold can be observed and therefore the integrator shows poor accuracy. The variational integrators (22), with $s \geq w$ holds, are stiffly accurate and thus they are the interesting ones. The degree w of λ_d determines the number $z = w + 1$ of the quadrature nodes of the Lobatto quadrature and thus the order $ordZ = 2z - 2 = 2w$.

Remark on boundary values problems Alternatively, instead of a given initial configuration q_0^0 and momentum p_0^0 at time point $t_0 = 0$, let's assume that the configurations at the endpoints $q_0^0 = q(t_0)$ and $q_N^0 = q(t_N)$ are given, like in optimal control problems, see, e.g., [16]. The configurations $q_0^1, \dots, q_0^{s-1}, q_k^i$, $k = 1, \dots, N-1$, $i = 0, \dots, s-1$, are determined by solving the discrete Euler-Lagrange equations in (22), just as the Lagrange multipliers $\lambda_0^1, \dots, \lambda_0^{w-1}, \lambda_k^i$, $k = 1, \dots, N-1$, $i = 0, \dots, s-1$, except for the Lagrange multipliers λ_0^0 and λ_N^0 at the time endpoints t_0 respectively t_N.

Remark on Theorem 1 One might think that even without condition 1 the problem of disparity of unknowns and discrete equations in one time step could be fixed by one of the following two possibilities. Either assuming that λ_0^0 is given as λ_0^0 is uniquely determined by the initial conditions q_0^0 and p_0^0 from the continuous Euler-Lagrange equations (3) or counting all discrete Euler-Lagrange equations for the entire time interval $[t_0, t_N]$. There are $N(w+s)+1$ unknowns versus $N(w+s)+1$ equations. But in both possibilities, the stiffly accurate condition lacks and without additional restrictions, linear dependence of the discrete Euler-Lagrange equations is a problem.

3.4 Conservation properties

In this section, the conservation properties of the constrained variational integrators are discussed. The symplecticity and the energy behaviour are demonstrated generally, meaning without considering Theorem 1 in Section 3.3. To show the discrete Noether-theorem, we assume that condition 1 in Theorem 1 holds. The symmetry is examined as a special property of the stiffly accurate variational integrators, constructed in this work by using the Lobatto quadrature for the approximation of the constraints integral.

3.4.1 Symplecticity and energy behaviour

Define $\bar{S}_d(q_0^0, q_N^0)$ as the sum of $\bar{L}_d$ in (**??**), i.e., $\bar{S}_d(q_0^0, q_N^0) = \sum_{k=0}^{N-1} \bar{L}_d(q_k^0, q_k^s)$, depending on the fixed boundaries values q_0^0 and q_N^0, where $\{q_k, \lambda_k\}$ is the solution of the discrete Euler-Lagrange equations (15). With the Legendre transforms (16), (17) the total differential reads

$$d\bar{S}_d = \frac{\partial \bar{S}_d}{\partial q_0^0} dq_0^0 + \frac{\partial \bar{S}_d}{\partial q_N^0} dq_N^0 = -p_0^0 dq_0^0 + p_N^0 dq_N^0$$

which is the basic formula for symplecticity generating functions, see [5]. Consequently, along the discrete solution $\{q_k^0, p_k^0\}$ provided by the variational integrators based on $\bar{S}_d(q_0^0, q_N^0)$ with p_k^0 calculated via the Legendre transforms (16), (17) the wedge product is conserved. In accordance with the general theory of symplectic integrators, variational integrators show a good energy behaviour.

3.4.2 Discrete Noether theorem

The continuous Noether theorem for constrained systems (see Section 2.1) can be extended to a discrete analog. It is assumed, that condition 1 of Theorem 1 holds.

We use the discrete Lagrangian $L_d(q_k^0, q_k^s)$, introduced in [17], that is characterized as follows

$$L_d(q_k^0, q_k^s) = \underset{\substack{q_k^\nu \in Q,\\ \nu \in \{1,\dots,s-1\}}}{\text{ext}} h \sum_{i=1}^{r} b_i L(q_d(c_i h; q_k), \dot{q}_d(c_i h; q_k)) \tag{30}$$

where the $(s-1)$ configurations $q_k^1, \dots, q_k^{s-1}$ are determined by extremizing the discrete Lagrangian.

Let Φ be a one-parameter group of transformations $\Phi = \{\phi_u : u \in \mathbb{R}\}$, leaving the Lagrangian L and the constraints manifold C invariant, see Section 2.1. Suppose, the one-parameter group Φ leaves the discrete Lagrangian $L_d(q_0^0, q_1^0)$ invariant, i.e., $L_d(\phi_u(q_0^0), \phi_u(q_1^0)) = L_d(q_0^0, q_1^0)$, $\forall (q_0^0, q_1^0) \in Q \times Q$, $\forall u \in \mathbb{R}$, then the first integral (5) is also an invariant of the constrained discrete Euler-Lagrange equations

$$I(q_0^0, p_0^0) = I(q_k^0, p_k^0) \qquad \forall \quad k = 1, \dots, N \tag{31}$$

The momentum p_k^0 is provided by the discrete Legendre transforms (16), (17).

The discrete Noether theorem for unconstrained systems is shown in [5] and can be applied to constrained systems when $g(\phi_u(q)) = 0$ $\forall q \in C$ holds. A proof of the discrete Noether theorem for constrained systems can be found in, e.g., [17].

The first integral (5) is only an invariant of the discrete Euler-Lagrange equations, if the discrete Lagrangian L_d inherits the invariance of the Lagrangian L, what is the case, when q_d is equivariant w.r.t. Φ, see [20].

3.4.3 Time reversibility

The flow of an autonomous Hamiltonian system is time reversible. Thus, the use of numerical methods that produce a time reversible numerical flow seems favorable. When using time reversible numerical methods, a long-time behaviour of the numerical solution similar to the exact solution is expectable [5]. The definition of time reversibility of a numerical method is taken from [5].

A numerical one-step method Φ_d is called symmetric or time reversible or self-adjoint, if it satisfies

$$\Phi_d^h \circ \Phi_d^{-h} = id \qquad \text{or equivalently} \qquad \Phi_d^h = (\Phi_d^{-h})^{-1} = (\Phi_d^h)^* \tag{32}$$

The method $(\Phi_d^h)^* = (\Phi_d^{-h})^{-1}$ is called the adjoint method.

In the following, the discrete Hamiltonian map $\tilde{F}_{\bar{L}_d} : T^*Q|_C \to T^*Q|_C$, i.e., the solution of (22) combined with the discrete Legendre transform yielding the mapping $\tilde{F}_{\bar{L}_d} : (q_k^0, p_k^0) \mapsto (q_{k+1}^0, p_{k+1}^0)$, its projection to the configuration space $\pi_Q \circ \tilde{F}_{\bar{L}_d}$ via $\pi_Q : T^*Q \to Q$, and its hidden constraint fulfilling variant $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$ are investigated. The adjoint discrete augmented Lagrangian $\bar{L}_d^* : Q^{s+1} \times (\mathbb{R}^m)^{w+1} \times \mathbb{R} \to \mathbb{R}$ of the discrete augmented Lagrangian $\bar{L}_d : Q^{s+1} \times (\mathbb{R}^m)^{w+1} \times \mathbb{R} \to \mathbb{R}$ is defined by

$$\bar{L}_d^*(q_0^0, \dots, q_1^0, \lambda_0^0, \dots, \lambda_1^0, h) = -\bar{L}_d(q_1^0, \dots, q_0^0, \lambda_1^0, \dots, \lambda_0^0, -h) \tag{33}$$

The discrete augmented Lagrangian $\bar{L}_d$ is self adjoint, when $\bar{L}_d^* = \bar{L}_d$ holds.

The following theorem connects the adjoint of the discrete augmented Lagrangian with the adjoint of the one step method $\tilde{F}_{\bar{L}_d}$.

Theorem 2 *(i) Adjointness: Let $\bar{L}_d^*$ be the adjoint of $\bar{L}_d$, then the projection of the adjoint method of $\tilde{F}_{\bar{L}_d}$ on Q is the projection of $\tilde{F}_{\bar{L}_d^*}$ on Q, i.e., $\pi_Q \circ \tilde{F}^*_{\bar{L}_d} = \pi_Q \circ \tilde{F}_{\bar{L}_d^*}$. If the momenta are forced to fulfill the hidden constraints, $\tilde{F}_{\bar{L}_d^*}$ is the adjoint method of $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$. (ii) Self-adjointness: If the discrete augmented Lagrangian is self-adjoint, then $\pi_Q \circ \tilde{F}^*_{\bar{L}_d} = \pi_Q \circ \tilde{F}_{\bar{L}_d}$ and $\tilde{F}_{\bar{L}_d}$ is called time reversible on configuration level. Under the additional assumption that the hidden constraints are fulfilled, $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$ is self-adjoint and thus time reversible on configuration and momentum level. Conversely, if $\tilde{F}_{\bar{L}_d}$ is time reversible or $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$ is self-adjoint, then the discrete augmented Lagrangian is equivalent to a self-adjoint discrete augmented Lagrangian.*

Proof. The adjoint method of the discrete Hamiltonian map $\tilde{F}_{\bar{L}_d}$ is studied by means of linear polynomials for q_d and λ_d and quadrature formulas of order two. In the linear case there are no intermediate nodes, i.e., $q_k = (q_k^0, q_k^1)$ respectively $\lambda_k = (\lambda_k^0, \lambda_k^1)$, and we denote q_k^0 by q_k and q_k^1 by q_{k+1} respectively λ_k^0 by λ_k and λ_k^1 by λ_{k+1}. The idea of the proof builds up on Theorem 2.4.1 in [17], there shown for the unconstrained case.

Consider the two discrete augmented Lagrangians $\bar{L}_d : Q \times Q \times \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}$ and $\bar{L}_d^* : Q \times Q \times \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}$

$$\bar{L}_d\left(q_0, q_1, \lambda_0, \lambda_1, h\right) = L_d\left(q_0, q_1, h\right) - \frac{h}{2}\left(g\left(q_0\right)\lambda_0 + g\left(q_1\right)\lambda_1\right) \tag{34}$$

$$\bar{L}_d^*(q_0, \bar{q}_1, \bar{\lambda}_0, \bar{\lambda}_1, h) = L_d^*(q_0, \bar{q}_1, h) - \frac{h}{2}(g(q_0)\bar{\lambda}_0 + g(\bar{q}_1)\bar{\lambda}_1) \tag{35}$$

and the corresponding discrete methods $\tilde{F}_{\bar{L}_d}$ and $\tilde{F}_{\bar{L}_d^*}$. Suppose $(q_1, p_1) \in T^*Q|_C$ are given.

(i) Replacing h by $-h$ and switching the roles of (q_0, p_0) and (q_1, p_1) in $\tilde{F}_{\bar{L}_d}$ reads

$$p_1 = -D_1\bar{L}_d(q_1, q_0, \lambda_1, \lambda_0, -h) \tag{36}$$

$$0 = g(q_0) \tag{37}$$

$$0 = D_2\bar{L}_d(q_1, q_0, \lambda_1, \lambda_0, -h) + D_1\bar{L}_d(q_0, q_{-1}, \lambda_0, \lambda_{-1}, -h) \tag{38}$$

$$0 = g(q_{-1}) \tag{39}$$

$$p_0 = D_2\bar{L}_d(q_1, q_0, \lambda_1, \lambda_0, -h) \tag{40}$$

and yields q_0, p_0, q_{-1}, λ_0, λ_1. The discrete method $\tilde{F}_{\bar{L}_d^*} : (q_0, p_0) \mapsto (\bar{q}_1, \bar{p}_1)$ is defined as

$$p_0 = -D_1\bar{L}_d^*(q_0, \bar{q}_1, \bar{\lambda}_0, \bar{\lambda}_1, h) \tag{41}$$

$$0 = g(\bar{q}_1) \tag{42}$$

$$0 = D_2\bar{L}_d^*(q_0, \bar{q}_1, \bar{\lambda}_0, \bar{\lambda}_1, h) + D_1\bar{L}_d^*(\bar{q}_1, \bar{q}_2, \bar{\lambda}_1, \bar{\lambda}_2, h) \tag{43}$$

$$0 = g(\bar{q}_2) \tag{44}$$

$$\bar{p}_1 = D_2\bar{L}_d^*(q_0, \bar{q}_1, \bar{\lambda}_0, \bar{\lambda}_1, h) \tag{45}$$

and yields $\bar{q}_1$, $\bar{p}_1$, $\bar{q}_2$, $\bar{\lambda}_0$, $\bar{\lambda}_1$.

Let $\bar{L}_d^*$ be the adjoint of $\bar{L}_d$ as defined in (33), with $s = w = 1$. Taking the derivatives of $\bar{L}_d^*$ yields

$$D_1 L_d^*(q_0, q_1, h) - \frac{h}{2} G^T(q_0)\lambda_0 = -D_2 L_d(q_1, q_0, -h) - \frac{h}{2} G^T(q_0)\lambda_0 \tag{46}$$

$$D_2 L_d^*(q_0, q_1, h) - \frac{h}{2} G^T(q_1)\lambda_1 = -D_1 L_d(q_1, q_0, -h) - \frac{h}{2} G^T(q_1)\lambda_1 \tag{47}$$

For $\tilde{F}_{\bar{L}_d}$ and $\tilde{F}_{\bar{L}_d^*}$ to be adjoint, the definition (32) requires that $\bar{p}_1 = p_1$ and $\bar{q}_1 = q_1$.

The initial values (q_0, p_0) in $\tilde{F}_{\bar{L}_d^*} : (q_0, p_0) \mapsto (\bar{q}_1, \bar{p}_1)$ are given by the solution of (36)–(40). Now (40) together with $q_1 \in C$ yields

$$p_0 = -D_1 L_d^*(q_0, q_1, h) + \frac{h}{2} G^T(q_0)\lambda_0 \tag{48}$$

$$0 = g(q_1) \tag{49}$$

while (41) and (42) read

$$p_0 = -D_1 L_d^*(q_0, \bar{q}_1, h) + \frac{h}{2} G^T(q_0)\bar{\lambda}_0 \tag{50}$$

$$0 = g(\bar{q}_1) \tag{51}$$

with the same (q_0, p_0). For h small enough, there exist unique solutions $\bar{q}_1, \bar{\lambda}_0$ and q_1, λ_0, thus $q_1 = \bar{q}_1 \in C$ and $\lambda_0 = \bar{\lambda}_0$ holds. Thus $\pi_Q \circ \tilde{F}_{\bar{L}_d}^* = \pi_Q \circ \tilde{F}_{\bar{L}_d^*}$. Using the definition in (33) in (36) yields

$$p_1 = D_2 L_d^*(q_0, q_1, h) - \frac{h}{2} G^T(q_1)\lambda_1 \tag{52}$$

while (45) reads

$$\bar{p}_1 = D_2 L_d^*(q_0, \bar{q}_1, h) - \frac{h}{2} G^T(\bar{q}_1)\bar{\lambda}_1 \tag{53}$$

Thus, checking the second requirement $\bar{p}_1 = p_1$ yields

$$-p_1 + \bar{p}_1 = \frac{h}{2} G^T(q_1)(\lambda_1 - \bar{\lambda}_1) \tag{54}$$

Equation (54) shows that $\tilde{F}_{\bar{L}_d^*}$ is not necessarily the adjoint of $\tilde{F}_{\bar{L}_d}$. The Lagrange multipliers λ_1 and $\bar{\lambda}_1$ might differ and therefore the momenta p_1 and $\bar{p}_1$ too, as $G^T(q_1)$ has full rank. The momenta p_1 and $\bar{p}_1$ only differ in the magnitude of the constraint force $G^T(q_1)$, i.e., in the normal direction, thus they are two representatives of the same equivalence class. To get the representative that fulfills the hidden constraints one can use the projection $\mathbb{P} : T^*Q|_C \to \eta(T^*C)$ in (4) and gets $\mathbb{P}p_1 = \mathbb{P}\bar{p}_1 \in \eta(T^*C)$ showing that $\tilde{F}_{\bar{L}_d^*}$ is the adjoint of $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$.

(ii) When $\bar{L}_d$ is self-adjoint, i.e., $\bar{L}_d^* = \bar{L}_d$

$$\pi_Q \circ \tilde{F}^*_{\bar{L}_d} \overset{\text{(i)}}{=} \pi_Q \circ \tilde{F}_{\bar{L}^*_d} = \pi_Q \circ \tilde{F}_{\bar{L}_d} \tag{55}$$

Furthermore, when additionally the momenta fulfill the hidden constraints, $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$ is self-adjoint.

Conversely, if $\pi_Q \circ \tilde{F}^*_{\bar{L}_d} = \pi_Q \circ \tilde{F}_{\bar{L}^*_d}$ the equations (48)–(51) hold with $\bar{q}_1 = q_1$ and $\bar{\lambda}_0 = \lambda_0$. As p_0 in (48) is equal to p_0 in (50), the derivatives of $\bar{L}_d$ and $\bar{L}^*_d$ with respect to q_0 satisfy the definition of adjointness (33) and therefore $\bar{L}_d$ and $\bar{L}^*_d$ are mutually adjoint up to the addition of a function of h. If $\tilde{F}_{\bar{L}_d}$ and $\tilde{F}_{\bar{L}^*_d}$ are adjoint, the momenta must fulfill the hidden constraints, and definition (32) implies the equations (48)–(53), with $\bar{q}_1 = q_1$, $\bar{\lambda}_0 = \lambda_0$, $\bar{p}_1 = p_1$, $\bar{\lambda}_1 = \lambda_1$. The momentum p_1 in (52) equals $\bar{p}_1$ in (53) and states that the derivatives of $\bar{L}_d$ and $\bar{L}^*_d$ with respect to q_1 also satisfy the definition of adjointness (33). Time reversibility on configuration level or self-adjointness of $\tilde{F}_{\bar{L}_d} : \eta(T^*C) \to \eta(T^*C)$ implies that $\bar{L}_d$ is equivalent to a self-adjoint discrete augmented Lagrangian. □

Remark on time reversibility of SHAKE Theorem 2 explains the reason for different statements in literature pertaining to the time reversibility of SHAKE. Regarding only the discrete flow of SHAKE on configuration level, the method can be stated to be symmetric, whereas the mapping $(q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$ is not symmetric, with p_{k+1} being the representative of the equivalence class $[p_{k+1}]$ provided by the SHAKE method. However, the discrete flow $(q_k, [p_k]) \mapsto (q_{k+1}, [p_{k+1}])$ is time reversible. One can choose the representative that does fulfill the hidden constraints by a projection step and the resulting (q_k, p_k) sequence is the same that is obtained by the RATTLE-algorithm, see [18]. The symmetry of RATTLE is shown in [13].

The proof of the Theorem 2 works analogously when higher degree polynomials and higher quadrature orders are used. Note that using linear polynomials for q_d and λ_d is the simplest case of the variational integrators (22). Finally it can be summarized that the projection π_Q of the adjoint of the discrete Hamiltonian map of $\bar{L}_d$ is the projection π_Q of the discrete Hamiltonian map of $\bar{L}^*_d$, with $\bar{L}^*_d$ being the adjoint discrete augmented Lagrangian of L_d. However, $\tilde{F}_{\bar{L}_d}$ and $\tilde{F}_{\bar{L}^*_d}$ are not necessarily adjoint due to the fact that the momenta are not forced to fulfill the hidden constraints. Furthermore, when $\bar{L}^*_d = \bar{L}_d$, the variational integrators are time reversible on configuration level and also on momentum level if the projection (4) is used in a postprocessing step to enforce the hidden constraints. Under which conditions $\bar{L}^*_d = \bar{L}_d$ is true, is shown next, based on [20].

Lemma 1 *Let $\bar{L}_d$ be the discrete augmented Lagrangian with symmetric quadrature formulas $(b_i, c_i)_{i=1}^r$ and $(e_i, f_i)_{i=1}^z$ and interpolation polynomials q_d and λ_d each with symmetrically distributed control points $(d_j)_{j=0}^s$ and $(\tilde{d}_j)_{j=0}^w$. Then $\bar{L}_d$ is self-adjoint.*

Proof. The following holds

$$q_d(-t;q_0,-h) = \sum_{\nu=0}^{s} q_0^{\nu} l_{\nu,s}\left(\frac{t}{h}\right) = q_d(t;q_0,h) \tag{56}$$

$$\dot{q}_d(-t;q_0,-h) = \frac{1}{-h}\sum_{\nu=0}^{s} q_0^{\nu} \dot{l}_{\nu,s}\left(\frac{t}{h}\right) = -\dot{q}_d(t;q_0,h) \tag{57}$$

$$\lambda_d(-t;\lambda_0,-h) = \sum_{\upsilon=0}^{w} \lambda_0^{\upsilon} l_{\mu,s}\left(\frac{t}{h}\right) = \lambda_d(t;\lambda_0,h) \tag{58}$$

The correlation between the Lagrange polynomials $l_{\nu,s}$ and $l_{s-\nu,s}$ and the Lagrange polynomials $\tilde{l}_{\mu,w}$ and $\tilde{l}_{w-\mu,w}$, with $\tau \in [0,1]$,

$$\begin{aligned} l_{\nu,s}(1-\tau) &= l_{s-\nu,s}(\tau) \\ \tilde{l}_{\mu,s}(1-\tau) &= \tilde{l}_{s-\mu,s}(\tau) \end{aligned}$$

is due to the symmetry of the control points d_j of q_d and the symmetry of the control points $\tilde{d}_j$ of λ_d. With $q_0 = (q_0^0,\ldots,q_0^s)$, $\tilde{q}_0 = (q_0^s,\ldots,q_0^0)$ and $t \in [0,h]$

$$q_d(t;\tilde{q}_0,h) = q_d(h-t;q_0,h) \tag{59}$$

The derivative reads

$$\dot{q}_d(h-t;q_0,h) = -\dot{q}_d(t;\tilde{q}_0,h) \tag{60}$$

Analogously, with $\lambda_0 = (\lambda_0^0,\ldots,\lambda_0^w)$ and $\tilde{\lambda}_0 = (\lambda_0^w,\ldots,\lambda_0^0)$, the polynomial $\lambda_d(t;\tilde{\lambda}_0,h)$ is rearrangeable to $\lambda_d(h-t;\lambda_0,h)$ via

$$\begin{aligned} \lambda_d(t;\tilde{\lambda}_0,h) &= \sum_{\mu=0}^{w} \lambda_0^{w-\mu}\tilde{l}_{\mu,w}\left(\frac{t}{h}\right) = \sum_{k=0}^{w} \lambda_0^{k}\tilde{l}_{w-k,w}\left(\frac{t}{h}\right) \\ &= \sum_{k=0}^{w} \lambda_0^{k}\tilde{l}_{k,w}\left(1-\frac{t}{h}\right) = \sum_{k=0}^{w} \lambda_0^{k}\tilde{l}_{k,w}\left(\frac{h-t}{h}\right) \\ &= \lambda_d(h-t;\lambda_0,h) \end{aligned} \tag{61}$$

Finally, (56) together with (59), respectively (57) with (60), (58) with (61), yields

$$q_d(-t;\tilde{q}_0,-h) = q_d(t;\tilde{q}_0,h) = q_d(h-t;q_0,h) \tag{62}$$

$$\dot{q}_d(-t;\tilde{q}_0,-h) = -\dot{q}_d(t;\tilde{q}_0,h) = \dot{q}_d(h-t;q_0,h) \tag{63}$$

$$\lambda_d(-t;\tilde{\lambda}_0,-h) = \lambda_d(t;\tilde{\lambda}_0,h) = \lambda_d(h-t;\lambda_0,h) \tag{64}$$

Substituting these expressions in the adjoint discrete augmented Lagrangian $\bar{L}_d^*$ shows that $\bar{L}_d$ is self-adjoint under the assumption of symmetric quadrature for-

mulas $(b_i, c_i)_{i=1}^{r}$ and $(e_i, f_i)_{i=0}^{w}$.

$$\begin{aligned}
-\bar{L}_d(\tilde{q}_0, \tilde{\lambda}_0, -h) =& -(-h)\sum_{i=1}^{r} b_i L(q_d(-c_i h; \tilde{q}_0, -h)), \dot{q}_d(-c_i h; \tilde{q}_0, -h)) \\
&+ (-h)\sum_{i=1}^{z} e_i [g(q_d(-f_i h; \tilde{q}_0, -h)) \cdot \lambda_d(-f_i h; \tilde{\lambda}_0, -h)] \\
=& h\sum_{i=1}^{r} b_i L(q_d(h - c_i h; q_0, h)), \dot{q}_d(h - c_i h; q_0, h)) \\
&- h\sum_{i=1}^{z} e_i [g(q_d(h - f_i h; q_0, h)) \cdot \lambda_d(h - f_i h; \lambda_0, h)] \\
=& h\sum_{i=1}^{r} b_{r+1-i} L(q_d(c_{r+1-i} h; q_0, h)), \dot{q}_d(c_{r+1-i} h; q_0, h)) \\
&- h\sum_{i=1}^{z} e_{z+1-i} [g(q_d(f_{z+1-i} h; q_0, h)) \cdot \lambda_d(f_{z+1-i} h; \lambda_0, h)] \\
=& \bar{L}_d(q_0, \lambda_0, h) \qquad (65)
\end{aligned}$$

Thus, $\bar{L}_d$ in (18) is self adjoint because the used quadrature formulas Lobatto and Gauss are symmetric and the control points of q_d and λ_d are chosen symmetrically. □

The corollary is that the higher order constrained variational integrators here are time reversible on configuration level, but not necessarily on momentum level. Numerical investigations confirm the results.

3.5 Relation to other methods for index 3 DAEs

In [17], Galerkin discrete Lagrangians are extended to include holonomic constraints. The Galerkin discrete Lagrangian is modified as follows

$$L_d(q_0, q_1, h) = \underset{\substack{q \in C^s([0,h],Q) \\ g(q(c_i h))=0}}{\operatorname{ext}} \sigma^s(q) \qquad (66)$$

whereby $g : Q \to \mathbb{R}$ is the constraint function and $\sigma^s(q)$ is the approximated action. The requirements $c_1 = 0$ and $c_s = 1$ stated in [17] constrain q_0 and q_1 to lie on the constraint submanifold. This is conform with the requirements mentioned in Section 3.3 to satisfy the stiffly accurate condition. However, in [17] no splitting of the two integrals in Lagrangian integral and constraints integral is made and thus diversity in approximation by using different quadrature formulas is not possible. Furthermore, in contrast to [17], the number of quadrature points is not restricted to be equal to the degree s of the polynomial q_d here.

Based on the discrete augmented Lagrangian $\bar{L}_d$ in (18) we can use the variational principle together with the Legendre transforms $p_k^0 = -D_1 \bar{L}_d(q_k, \lambda_k)$ and

$p^0_{k+1} = D_{s+1}\bar{L}_d(q_k, \lambda_k)$ to set up the following discrete equations

$$
\begin{aligned}
p^0_k &= -D_1\bar{L}_d(q_k,\lambda_k) = -D_1 L_d(q_k) + h\sum_{i=0}^{w-1} e_{i+1}G^T(q_d(\tilde{d}_i h))l_{0,s}(\tilde{d}_i)\lambda^i_k \\
0 &= D_\nu\bar{L}_d(q_k,\lambda_k) = D_\nu L_d(q_k) - h\sum_{i=1}^{w-1} e_{i+1}G^T(q_d(\tilde{d}_i h))l_{\nu-1,s}(\tilde{d}_i)\lambda^i_k \quad \nu = 2,\dots,s \\
p^0_{k+1} &= D_{s+1}\bar{L}_d(q_k,\lambda_k) = D_{s+1}L_d(q_k) - h\sum_{i=1}^{w} e_{i+1}G^T(q_d(\tilde{d}_i h))l_{s,s}(\tilde{d}_i)\lambda^i_k \\
0 &= g(q_d(\tilde{d}_i h)) \quad i = 1,\dots,w
\end{aligned}
\tag{67}
$$

For given q^0_k and p^0_k the set of equations (67) shows a discrepancy between the number of unknowns $(s+w+2)$ and the number of equations $(s+w+1)$, because the Lagrange multiplier λ^w_k enters into the update of p^0_{k+1}. To solve the system of equations, an additional equation, that is not naturally obtained by the variational principle, is required. As a remedy, the update p^0_{k+1} can be extended by a projection step, choosing λ^w_k such that (q^0_{k+1}, p^0_{k+1}) lie on the manifold $\eta(T^*_{q^0_{k+1}}C)$. This was first suggested by Anderson (1983) and yielded the RATTLE algorithm [5]. Construction methods to show the equivalence of variational integrators and symplectic Runge-Kutta methods for unconstrained systems are given in [17] and in a more general way in [5]. Extending these approaches to the constrained case, it can be shown that for $r = s$ the set of equations (67) together with the projection step can be rearranged to a discrete Hamiltonian map $(q^0_k, p^0_k) \mapsto (q^0_{k+1}, p^0_{k+1})$ that is a constrained symplectic partitioned Runge-Kutta method identical to the ones introduced by [10], [11], [12] and studied in, e.g., [17]. They are called symlectic SPARK-methods. As stated in [12], they are variational integrators. This is shown in [12] and mentioned in [17]. In [12] the generating function of the symplectic SPARK integrators is defined by

$$
A_d(q_0, q_1, h) := h\sum_{i=1}^{s} b_i L(Q_i, V_i) - h\sum_{i=0}^{\tilde{s}} \tilde{b}_i \Lambda_i g(\tilde{Q}_i) \tag{68}
$$

The number of quadrature nodes used to approximate the Lagrangian integral and the degree of the polynomial q_d are both s in (68). This is in contrast to the variational integrators presented here. The number r of the quadrature nodes of the quadrature formula $(c_i, b_i)_{i=1}^r$ is not restricted to s. Numerical investigations reveal that when using the Lobatto-quadrature to approximate the integral of the Lagrangian in (18) the choice of the degree s of q_d to be one less than the number of quadrature points r yields a more efficient integrator compared to the established combination $r = s$. In particular we get the same convergence orders for the two combinations while one unknown less has to be solved for in the discrete Euler-Lagrange equations (22) in the first mentioned combination. Note for $r > s$ the construction method given in [5] for the equivalence of variational integrators and symplectic Runge-Kutta methods fails, as the internal stage derivatives V_i become linearly dependent, see [19] for further details. However, following the approach in [19], it is possible to derive a so called modified constrained symplectic Runge-Kutta method [25]. There is another important difference. The variational integrators introduced in this paper go along with a continuous discrete trajectory

$\{\lambda_k\}_{k=0}^{N-1}$, since $\lambda_k^w = \lambda_{k+1}^0$. In contrast to the symplectic SPARK integrators, that go along with a discontinuous trajectory, since $\lambda_k^w \neq \lambda_{k+1}^0$ [23]. In particular, choose $s = w$, $ordL = 2s$ (Gau), $ordZ = 2w$ (Lob) to determine the generating function $\bar{L}_d$ (18). Then, the associated discrete Hamiltonian map, i.e., the discrete equations in (67) together with the projection step, is equal to the symplectic (s, s)-Gauss-Lobatto SPARK method [12] applied to an overdetermined DAE of index 2. When setting $w = s - 1$, $ordL = 2s - 2$ (Lob), $ordZ = 2s - 2$ (Lob) the associated discrete Hamiltonian map to (18) is the constrained Lobatto IIIA-IIIB method [11], [17].

Approximating the constraints integral via the Gauss quadrature (24), in addition using the Gauss quadrature for the approximation of the Lagrangian integral as well, with $w = s + 1$, $ordL = 2s$ (Gau), $ordZ = 2s$ (Gau), the associated discrete Hamiltonian map is the s-stage Gauss method applied to an index 3 DAE. Investigations in [3] already show, that the Gauss method is rather inappropriate for this type of application, due to not being stiffly accurate.

4 Numerical Analysis

The performance and the convergence order of the variational integrators (22) are examined and demonstrated by means of two numerical examples. The investigated numerical examples are the planar pendulum and the three-dimensional double pendulum.

The motion of the planar pendulum is described by redundant coordinates $q = [x, y]^T \in \mathbb{R}^2$. The constraint function g

$$g = \frac{1}{2}(x^2 + y^2 - l^2)$$

constrains the motion to the submanifold $C = \mathbb{S}_l^1$, whereby l is the rod length. With mass m, yielding the $[2 \times 2]$ mass matrix $M = mI_{2\times 2}$, and with the gravitation $g = [0, -9.81]^T$, the Lagrangian reads

$$L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} + (Mg)^T \cdot q \tag{69}$$

The second dynamical system, the three-dimensional double pendulum, has the configuration space $Q = \mathbb{R}^6$, with $q = [x_1, y_1, z_1, x_2, y_2, z_2]^T$. The configuration space is constrained to the submanifold $C = g^{-1}(0)$, with $g = [g_1, g_2]^T$,

$$g_1 = \frac{1}{2}(x_1^2 + y_1^2 + z_1^2 - l_1^2)$$
$$g_2 = \frac{1}{2}((x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2 - l_2^2)$$

with rod lengths l_1, l_2. With the pendulum masses m_1, m_2, yielding the $[6\times 6]$ mass matrix M and with the gravitation $g = [0, 0, -9.81, 0, 0, -9.81]^T$ the Lagrangian is also given in (69). As shown in Section 3.3, the number of admissible combinations of the degrees s of q_d and w of λ_d and the quadrature formulas $(c_i, b_i)_{i=1}^r$ of order $ordL$ and $(e_i, f_i)_{i=1}^z$ of order $ordZ$ is restricted. A short review is given here. For the approximation of the constraints integral only the Lobatto quadrature is used and the degree w of the polynomial λ_d is coupled to the order of the quadrature formula via $ordZ = 2w$. Additionally, the inequality $w \leq s$ has to be satisfied. All other combinations fulfilling this are tested.

Table 1 Convergence orders of the variational integrator (22) for q, p, λ
$L_d(q_k)$ (19) approximated via **Gauss** quadrature of order oL, where $oL = ordL$
$g_d(q_k, \lambda_k)$ (20) approximated via Lobatto quadrature of order oZ, where $oZ = ordZ$
s - degree of polynomial q_d, w - degree of polynomial λ_d

		oL	**2**	**4**	**6**	**8**	**10**	**12**	**4**	**6**	**8**	**10**	**12**	**6**	**8**	**10**	**12**	**8**	**10**	**12**	**10**	**12**	**12**
oZ	w	s	**1**	**1**	**1**	**1**	**1**	**1**	**2**	**2**	**2**	**2**	**2**	**3**	**3**	**3**	**3**	**4**	**4**	**4**	**5**	**5**	**6**
2	**1**	q	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
		p	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
		λ	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
4	**2**	q							4	4	4	4	4	4	4	4	4	2	2	2	2	2	2
		p							4	4	4	4	4	4	4	4	4	2	2	2	2	2	2
		λ							2	2	2	2	2	2	2	2	2	d	d	d	d	d	d
6	**3**	q												6	6	6	6	6	6	6	4	4	2
		p												4	4	4	4	4	4	4	2	2	2
		λ												4	4	4	4	4	4	4	2	2	d
8	**4**	q																8	8	8	8	8	6
		p																6	6	6	6	6	4
		λ																4	4	4	4	4	2
10	**5**	q																			10	10	10
		p																			6	6	6
		λ																			6	6	6
12	**6**	q																					12
		p																					8
		λ																					6

Table 2 Convergence orders of the variational integrator (22) for q, p, λ
$L_d(q_k)$ (19) approximated via **Lobatto** quadrature of order oL, where $oL = ordL$
$g_d(q_k, \lambda_k)$ (20) approximated via Lobatto quadrature of order oZ, where $oZ = ordZ$
s - degree of polynomial q_d, w - degree of polynomial λ_d

		oL	**2**	**4**	**6**	**8**	**10**	**12**	**2**	**4**	**6**	**8**	**10**	**12**	**4**	**6**	**8**	**10**	**12**	**6**	**8**	**10**	**12**	**8**	**10**	**12**	**10**	**12**
oZ	w	s	**1**	**1**	**1**	**1**	**1**	**1**	**2**	**2**	**2**	**2**	**2**	**2**	**3**	**3**	**3**	**3**	**3**	**4**	**4**	**4**	**4**	**5**	**5**	**5**	**6**	**6**
2	**1**	q	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
		p	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
		λ	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
4	**2**	q							2	4	4	4	4	4	4	4	4	4	4	2	2	2	2	2	2	2	2	2
		p							2	4	4	4	4	4	4	4	4	4	4	2	2	2	2	2	2	2	2	2
		λ							d	2	2	2	2	2	2	2	2	2	2	d	d	d	d	d	d	d	d	d
6	**3**	q													4	6	6	6	6	6	6	6	6	4	4	4	2	2
		p													2	4	4	4	4	4	4	4	4	2	2	2	2	2
		λ													2	4	4	4	4	4	4	4	4	2	2	2	d	d
8	**4**	q																		6	8	8	8	8	8	8	6	6
		p																		4	6	6	6	6	6	6	4	4
		λ																		2	4	4	4	4	4	4	2	2
10	**5**	q																						8	10	10	10	10
		p																						4	6	6	6	6
		λ																						4	6	6	6	6
12	**6**	q																									10	12
		p																									6	8
		λ																									4	6

4.1 Convergence order

The convergence order of the variational integrators (22) is investigated numerically. Using a constant step size over a fixed time interval, the convergence order is determined from the difference of the global errors for different step sizes. The global error e_g is obtained by the comparison of the simulated values to appropriate reference values, whereby x can be q, p, λ.

$$e_g = \max_{k\in\{0,\dots,N\}} \left\| x_k^0 - x_{ref}(kh) \right\|$$

The convergence orders of the configuration q, the Lagrange multiplier λ and the momentum p are examined. The Tables 1 and 2 show the results. The letter 'd' in the Tables stands for divergent, meaning the global error does not decrease when the time step decreases.

The convergence orders are discussed qualitatively. When $ordL$ becomes less than $2s$ using the Gauss quadrature respectively $2s-2$ using the Lobatto quadrature for calculating L_d in (19), the simulation does not work properly. No orders are listed for these cases. The two statements can be reformulated to one, saying the number of quadrature nodes r has to be greater or equal than s, i.e., $r \geq s$. The statement, observed here only numerically, is valid for an unconstrained dynamical system with a regular Lagrangian of the form $L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M\dot{q} - V(q)$, symmetric positive-definite mass-matrix M and ∇V being Lipschitz continuous, see [6] and [20]. In [6] it is shown that the discrete Lagrangian flow is well posed, when the order of the quadrature rule, that approximates the integral of the Lagrangian, is at least $2s-1$, meaning $r \geq s$ for the Gauss quadrature and $r \geq s+1$ for the Lobatto quadrature. However, the condition is only sufficient but not necessary as the standard Lobatto IIIA-B partitioned Runge-Kutta method is a counterexample with Lobatto quadrature of order $2s-2$ or rather $r = s$, see [20].

The following remarks are valid only for the gray shaded combinations in the Tables 1 and 2, i.e., $s = w$ and $s = w+1$. The results for the convergence order of the configuration q, briefly named $\mathrm{ord}(q)$, can be summarized as follows. It must be differentiated between calculating L_d in (19) via the Lobatto or via the Gauss quadrature.

L_d via Gauss quadrature	$\mathrm{ord}(q) = \min(ordL, ordZ) = \min(2s, 2r, 2w)$
L_d via Lobatto quadrature	$\mathrm{ord}(q) = \min(ordL, ordZ) = \min(2s, 2r-2, 2w)$

Thus, the orders $ordL$ and $ordZ$ of the quadrature formulas determine the resulting order of the variational integrator in q. Furthermore, the configuration q is super convergent of order $2s$, when $r \geq s$ (approximating L_d via the Gauss quadrature) respectively $r \geq s+1$ (approximating L_d via the Lobatto quadrature). The order of the Lagrange multiplier λ, $\mathrm{ord}(\lambda)$, is reduced compared to the order of the configuration q. The convergence order of the momentum p, $\mathrm{ord}(p)$, is mostly also smaller than the one of the configuration q. Note that the momentum p is calculated in a post-processing step via the discrete Legendre transform using the simulated configurations q and Lagrange multipliers λ. There is a relation between the degree w of the polynomial λ_d and the convergence orders of the Lagrange multiplier λ and the momentum p recognizable, again only valid for $s = w$ or

$s = w + 1$ and $ordL \geq 2s$.

w even	$\mathrm{ord}(p) = w + 2$	$\mathrm{ord}(\lambda) = w$
w uneven	$\mathrm{ord}(p) = w + 1$	$\mathrm{ord}(\lambda) = w + 1$

Furthermore, the relation $\mathrm{ord}(p) = \mathrm{ord}(q) - \mathrm{ord}(\lambda) + 2$ between the convergence orders of p and λ and q can be observed. Moreover it is significant, that all orders are even. The order of a symmetric integrator is even [5]. In Section 3.4.3 the symmetry of the variational integrators (22) is discussed. The variational integrators (22) are symmetric in q, but not in p and in λ. Nevertheless, the numerical examination reveals even orders for q, p and λ.

In order to achieve the same convergence order for p as for q, one may project the numerical solution onto $\eta(T^*_{q^0_k}C)$ via $p^{0,p}_k = \mathbb{P}p^0_k$, $k = 1, \ldots, N-1$, using the projection $\mathbb{P}$ in (4). The accuracy of the Lagrange multiplier can be improved if $\lambda^{0,p}_k$ is defined as

$$\lambda(q,p) = \left(GH^T_{pp}G^T\right)^{-1}\left(G_q\left(H^T_p, H^T_p\right) + GH^T_{pq}H^T_p - GH^T_{pp}H^T_q\right)(p,q) \qquad (70)$$

evaluated at q^0_k and $p^{0,p}_k$. The indices q and p denote the derivative w.r.t. q respectively p. Equation (70) is obtained by differentiating the constraints g two times w.r.t. t, supposing that $\left(GH^T_{pp}G^T\right)$ is invertible in a neighbourhood of the exact solution. Then the convergence order of λ is the same as the convergence orders of q and p. This approach for recalculating λ is suggested in [10]. In this work the improvement of the orders of p and λ is tested numerically only.

Order reduction of the Lagrange multiplier and the momentum is a known problem when integrating DAEs in Hessenberg-form of index 3, see, e.g., [4], [8], [3], [9]. In [3] the s-stage Radau IIA method is studied, the paper of [8] deals with the equivalent collocation method Radau IIA, both with regard to DAEs in Hessenberg form of index 3. The s-stage Radau IIA method, i.e., the collocation method Radau IIA, is stiffly accurate, but not symplectic. It is shown in [8], the Radau IIA-method applied to a DAE in Hessenberg-form, index 3, yields staggered orders, beginning with the order of the configuration q, i.e., $2s-1$, the order of the momentum decreases to s and the order of λ to $s-1$. Similar results pertaining to the reduction of the orders are obtained, when using the Gauss-method or Lobatto IIIC to approximate the solution of a DAE index 3 system [4], [9]. The (s,s)-SPARK Gauss-Lobatto integrators have the convergence order $2s$ both for the configuration q and the momentum p. The constrained Lobatto IIIA/IIIB method has a convergence order of $2s-2$. There is no order reduction in p due to the projection step on the manifold $\eta(T^*C)$. The DAEs of index 3 together with the constraints differentiated once w.r.t. t can be interpreted as a system of index 2 overdetermined DAEs [12]. To get accurate values for the Lagrange multiplier, the possibility given in [10] is to determine λ^w_k via the additional constraint (70). Then the convergence order of λ is the same as the convergence orders of q and p.

The combinations in the Tables 1 and 2, which are not shaded gray, show order reduction in q, p and λ. The increase of the degree s of the polynomial q_d to a value greater than $w+1$ comes along with decreased orders. The limitation of the order $ordZ$ to $2w$ might be a reason.

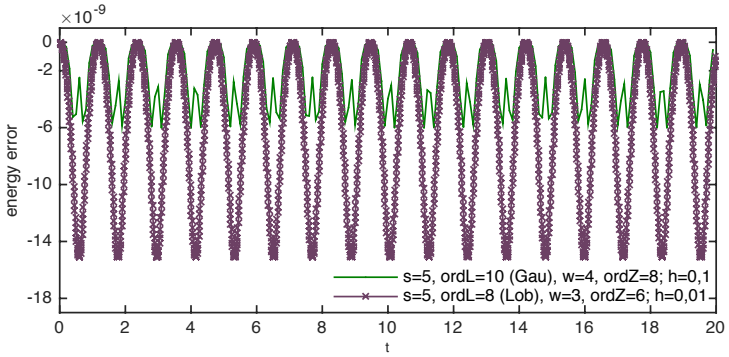

Fig. 2 Planar pendulum: Error of the total energy

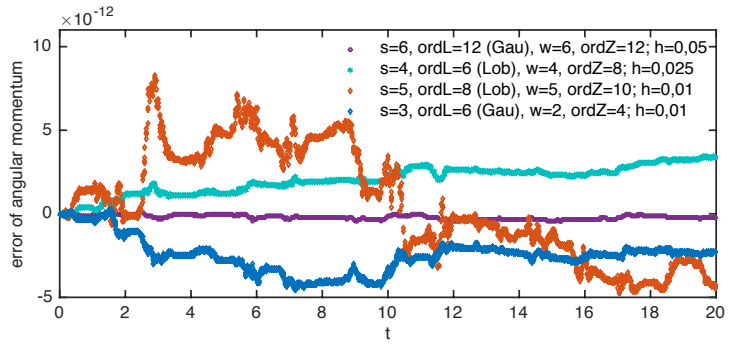

Fig. 3 Double pendulum: Error of the z-component of the angular momentum

4.2 Long-time energy behaviour and conservation of angular momentum

The variational integrators in (22) are symplectic and therefore show a good long-time energy behaviour, see Section 3.4.1. In Fig. 2 the error of the total energy of the planar pendulum is shown. The combinations $[s = 5, ordL = 10(\text{Gau}), w = 4, ordZ = 8]$ with $\text{ord}(q) = 8$ (see Table 1) and $[s = 5, ordL = 8(\text{Lob}), w = 3, ordZ = 6]$ with $\text{ord}(q) = 4$ (see Table 2) are chosen as representatives. Note, that in Fig. 2 the time step for the first mentioned combination is ten time larger than for the second and still the energy error is smaller. The error of the total energy decreases, when the order $\text{ord}(q)$ of the variational integrator increases. The same behaviour of the error of the total energy is given in case of the three-dimensional double pendulum. The use of the variational integrators leads to a stable energy behaviour. The error in Fig. 2 is oscillating, but stays bounded. The total energy of the system does not increase or decrease artificially over time. In the combination $[s = 5, ordL = 8(\text{Lob}), w = 3, ordZ = 6]$, s is not in the ideal ratio of s and w and therefore the order $\text{ord}(q)$ is reduced and the error of the total energy oscillates with greater amplitude. The Lagrangian of the double pendulum (69) is invariant under the group of rotations. Consequently the z-component of the angular momentum

$$I(p, q) = -p_{x1}y_1 + p_{y1}x_1 - p_{2x}y_2 + p_{2y}x_2 \tag{71}$$

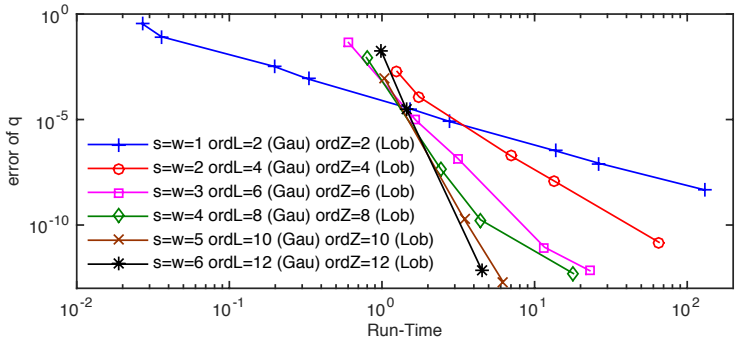

Fig. 4 Planar pendulum: Global error of the configuration q against run-time for the integrators $s = w = r = 1, \dots 6$, $OrdL = 2r$ (Gau), $OrdZ = 2w$ (Lob)

is a conserved quantity in the system, whereby $p_\alpha = (p_{\alpha x}, p_{\alpha y})$ denotes the momentum of the α-th mass, $\alpha = 1, 2$. As shown in Section 3.4.2 the augmented discrete Lagrangian $\bar{L}_d$ inherits the invariance of $\bar{L}$, when the group of transformations is linear. Thus, the variational integrators (22) conserve the z-component of the angular momentum. Fig. 3 shows the error of the z-component of the angular momentum for some combinations. The angular momentum is preserved up to numerical accuracy.

4.3 Computational efficiency

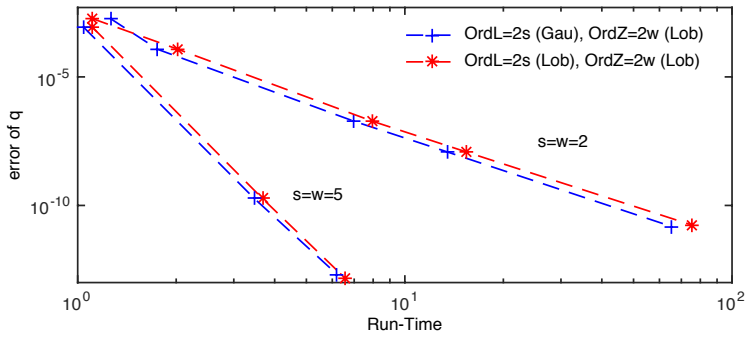

Fig. 5 Planar pendulum: Global error of the configuration q against run-time for the integrators $s = w$, $OrdL = 2s$ (Gau) respectively (Lob), $OrdZ = 2w$ (Lob)

To assess the computational efficiency of the variational integrators in (22), the error of the configuration q for different step sizes h is plotted versus the run-time. The parameters are chosen such that the oscillation period of the pendulum is an integer multiple of the time step size, such that the error of the simulation can be computed with respect to destined analytically known reference configu-

rations. Investigated are these integrators that have super convergence of $2s$ in q together with a minimal number of quadrature nodes. In particular, the combinations showed in Fig. 4 are $s = w = r = 1, \ldots, 6$ with the Gauss quadrature of order $2r$ for approximating the Lagrangian integral. The computational effort of the constrained higher order integrators reduces significantly and the results are much more accurate compared to the constrained integrator of order 2, i.e., the combination s = w = r = 1. Thus, increasing the order of the integrators yields higher accuracy while run time decreases.

When approximating the Lagrangian integral via the Lobatto quadrature, the minimal number of quadrature nodes r to achieve convergence order of $2s$ in q is $s + 1$. Thus, it is larger by one than using the Gauss quadrature. The evaluation of the Lagrangian at a further quadrature node costs run-time. Fig. 5 shows the influence by means of the combinations $s = w = 2$ and $s = w = 5$. For the same step sizes, the integrators provide the same accuracy, but the integrators that use the Gauss quadrature for approximating the Lagrangian integral are slightly faster than the ones using the Lobatto quadrature.

5 Conclusion

In this work, variational integrators of higher order for systems with holonomic constraints are constructed and analyzed. The idea is based on [20], where variational integrators of higher order for unconstrained systems have been constructed and analyzed, and on the constrained Galerkin methods, that are presented in [17]. The continuous curves q and λ are discretized via polynomials of degree s respectively w and quadrature rules of higher order are used to approximate the action integral. The distinction between the integral of the Lagrangian and the integral of the scalar product of the constraints and the Lagrange multipliers $g(q) \cdot \lambda$ allows the use of different quadrature formulas for each with r quadrature nodes for approximating the first and z for approximating the second. This is in contrast to the constrained Galerkin methods in [17]. Restrictions such that the control points of λ_d are disposed like the quadrature nodes z, in particular like the quadrature nodes of the Lobatto quadrature with $z = w + 1$, and $s \geq w$, ensure the solvability of the constrained discrete Euler-Lagrange equations and stiff accuracy. The resulting discrete augmented Lagrangian can serve as a generating function for the symplectic SPARK integrators of [12]. However, in [12] the symplectic SPARK integrator is applied to a system of index 2 overdetermined DAEs. Furthermore, contrary to [17] and [12] the restriction $r = s$ quadrature nodes for approximating the integral of the Lagrangian is dropped here as it is in [20] for the unconstrained systems. The preservation properties of the variational integrators, such as symplecticty and preservation of momentum maps, are proved analytically and verified numerically. It is shown that the presented variational integrators are time reversible on configuration level but not on momentum level because the momenta do not fulfill the hidden constraints. However, if the momenta are forced to fulfill the hidden constraints via a simple projection in a post processing step, the discrete flow is time reversible on configuration and momentum level. Note that this is achieved in a simpler way compared to symplectic SPARK integrators, where an additional equation and unknown is introduced to fulfill the hidden constraints. The order of convergence is determined numerically. The numerical investigations give a first

insight what orders can be expected for the configuration q, the Lagrange multiplier λ and the momentum p. The orders of the momentum and the Lagrange multiplier are reduced compared to the order of the configuration. Again, with a simple post processing step accomplishing the fulfillment of the hidden constraints, the order reduction can be avoided, while the symplectic SPARK integrators yield same orders of convergence for the configuration and the momentum [12] via solving an extended system of equations and unknowns. The numerical tests reveal highest orders for $r \geq s+1$, when the Lobatto quadrature is applied, and $r \geq s$ when the Gauss quadrature is applied. Furthermore, an increase of s to $s > w+1$ decreases the resulting orders. Inserting the coefficients of the Lobatto-quadrature for $(c_i, b_i)_{i=1}^{r}$ and choosing the degree of the polynomial q_d to be one less than r the resulting integrator has the same convergence order as when we choose the degree of q_d and r to be equal. However, the lower degree polynomial leads to one unknown less in the discrete Euler-Lagrange equations to be solved for and thus saves computational costs. Note, that for $r > s$ the constrained variational integrator is equivalent to a so called modified constrained symplectic Runge-Kutta method, that is an extension of the modified symplectic Runge-Kutta method in [19] to the holonomically constrained case. In view of highest accuracy and low computational effort, the most promising combinations are $s = w$ with $r = s$ (Gauss) or $r = s+1$ (Lobatto). A numerical investigation regarding efficiency versus accuracy is performed for these combinations, revealing that higher orders increase the accuracy substantially while the run-times decrease. Furthermore, at the same order of accuracy, the additional quadrature node being necessary using the Lobatto quadrature leads to a slightly higher run-time than using the Gauss quadrature.

The analytical proof of the convergence orders is future work. To decrease rounding off errors, a reformulation of the system of equations can be considered similar to the leap frog method. Note that the leap frog method results from a reformulation of SHAKE [17], which is a special case of the variational integrators presented here. Moreover the influence of using different interpolations methods for q_d, like, e.g., Chebyshev polynomials, could be investigated. The conditions that guarantee stiff accuracy include the restriction to choose a quadrature formula with the last quadrature node to be 1, which is satisfied by the Radau-IIA quadrature, too. First numerical tests using the Radau-IIA quadrature to approximate the integral of the scalar product $g(q) \cdot \lambda$ are promising. Moreover, in contrast to assuming the Lagrange multiplier λ_0^0 to be unknown, the initial conditions q_0^0, p_0^0 could be extended by it, such that the number of discrete Euler-Lagrange equations for one time step equal the number of unknowns. But this has to be investigated carefully, because without appropriate restrictions, linear dependence can occur and the lack of the stiffly accurate condition can lead to drift-off problems. The appliance of the variational integrators to more complex constrained systems is a next step, especially interesting for constrained systems that involve slow and fast time scales [15]. Another possible direction is to use the presented integrators for mechanical systems on selected Lie groups [1] embedded in the Euclidean space by constraints. Furthermore, reducing the dimension of the nonlinear equation system is another challenging topic. One could think of applying the nullspace method [14] on a specific type of the presented integrators, such that the dimension reduces from $(sn + wm)$ to sn.

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