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Structure-preserving integrators for constrained mechanical systems in the framework of the GGL principle

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Simulating multi-body systems often requires an appropriate treatment of the differential-algebraic equations (DAEs). The recently proposed *GGL principle* considers constraints both on configuration and on velocity level and embodies an index-reduction technique in the spirit of the often-applied GGL stabilization. In sharp contrast to the original formulation, the Euler-Lagrange equations of the GGL principle, fit into the Hamiltonian framework of mechanics. Therefore, the GGL principle facilitates the design of structure-preserving integrators. Due to the close relationship of the GGL principle to optimal control, previously developed direct methods can be used to obtain variational integrators for constrained mechanical systems. Furthermore, slight modifications can be applied to obtain second-order energy-momentum consistent integrators emanating from the GGL principle, which represent another important class of structure-preserving time-stepping schemes. The newly devised schemes circumvent issues of standard methods and provide more realistic results by accounting for velocity level constraints.

1 Introduction

A systematic approach for simulating multi-body systems lies in the choice of redundant coordinates $q(t) \in \mathbb{R}^n$ and corresponding velocities $\dot{q} \in \mathbb{R}^n$. We assume that the system has a seperable Lagrangian $L(q,\dot{q}) = T(\dot{q}) - V(q) = \frac{1}{2}\dot{q}\cdot M\dot{q} - V(q)$, where the kinetic energy T makes use of a constant, symmetric and positive definite mass matrix M and the potential energy is denoted by V. A corresponding Hamiltonian is given by $H(q,p) = T(p) + V(q)$ with conjugate momenta $p \in \mathbb{R}^n$ obtained by a Legendre transformation. The motion of the underlying system is restricted by m independent, scleronomic, holonomic constraints $g : \mathbb{R}^n \to \mathbb{R}^m$ which have to be fulfilled, viz.

$$g(q) = 0. \tag{1}$$

Since these position level constraints (sometimes referred to as *primary constraints*) have to hold at any time, hidden constraints $g^v : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^m$ are induced on velocity level as

$$\frac{\mathrm{d}}{\mathrm{d}t} g(q) = \mathrm{D}g(q)\dot{q} = 0 \quad \Rightarrow g^v(q,\dot{q}) = 0. \tag{2}$$

Consequently, the governing equations of motion are given by a set of differential-algebraic equations (DAEs), which have to be treated appropriately. By augmenting the Lagrangian, the set of equations can be obtained by Hamilton's principle

$$\delta \int_0^T L^\lambda(q,\dot{q})\,\mathrm{d}t = 0, \tag{3}$$

where the augmented Lagrangian $L^\lambda : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ introduces Lagrange multipliers $\lambda \in \mathbb{R}^m$ to enforce primary constraints (1) such that

$$L^\lambda(q,\dot{q}) = L(q,\dot{q}) - \lambda \cdot g(q). \tag{4}$$

Alternatively, a Hamiltonian approach can be chosen. The corresponding augmented Hamiltonian $H^\lambda : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ is given by

$$H^\lambda(q,p) = H(q,p) + \lambda \cdot g(q). \tag{5}$$

Eventually, the constrained dynamical system is governed by the canonical Hamiltonian DAEs, which read

$$\dot{q} = M^{-1}p, \tag{6a}$$
$$\dot{p} = -\mathrm{D}V(q), \tag{6b}$$
$$0 = g(q) \tag{6c}$$

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or more briefly in state space representation

$$\dot{z} = \mathbb{J}\mathrm{D}H^{\lambda}(z), \tag{7a}$$
$$0 = g(q), \tag{7b}$$

where the state space vector $z = (q, p) \in \mathbb{R}^{2n}$ is introduced along with the symplectic structure matrix $\mathbb{J} \in \mathbb{R}^{2n\times 2n}$. However, those DAEs are often prone to numerical ill-conditioning, since they have a differentiation index $\nu_{\mathrm{d}} = 3$. A straightforward way to circumvent those issues is to replace the positional constraints with the corresponding velocity level constraints, yielding index-2 DAEs. This, however, leads to drift phenomena in the original primary constraints. Thus, more commonly used index-reduction techniques, such as the well-known Gear-Gupta-Leimkuhler (GGL) stabilization (cf. Gear et al. [4]), are employed. By directly coupling the secondary constraints into the equations and modifying the kinematic relation (6a) an extented set of equations with index $\nu_{\mathrm{d}} = 2$ is obtained, given by

$$\dot{q} = M^{-1}p + \mathrm{D}g(q)^{\mathrm{T}}\gamma, \tag{8a}$$
$$\dot{p} = -\mathrm{D}V(q), \tag{8b}$$
$$0 = g(q), \tag{8c}$$
$$0 = \mathrm{D}g(q)M^{-1}p. \tag{8d}$$

However, these equations do not arise from a variational principle. Consequently, the Hamiltonian structure has been lost due to the direct modification of the equations of motion and one cannot find an underlying augmented Hamiltonian anymore. This furthermore leads to the problem, that crucial conservation properties are only fulfilled if the newly introduced Lagrange multiplier γ vanishes identically. This can be shown for the time-continuous set of equations (8) but will not hold in a time-discrete setting. Thus, the design of structure-preserving integration schemes can be difficult and often times numerical schemes discretizing the GGL equations (8) are not structure-preserving.

2 GGL principle

In this section, we want to focus on the recently presented GGL variational principle (cf. Kinon & Betsch [1]). It can be viewed as an extension of the *Livens principle* (cf. Livens [2] and Pars [3]), which is sometimes also referred to as *Hamilton-Pontryagin principle* (cf. Bou-Rabee & Marsden [9]). Livens principle introduces independent velocities $v \in \mathbb{R}^n$ by enforcing the kinematic relation by means of Lagrange multipliers $p \in \mathbb{R}^n$. Consequently, the mixed action integral reads

$$S(q, v, p) = \int_0^T (L(q, v) + p \cdot (\dot{q} - v))\,\mathrm{d}t. \tag{9}$$

Enforcing stationarity of the action integral yields the corresponding Euler-Lagrange equations as

$$\dot{q} = v \tag{10a}$$
$$\dot{p} = \mathrm{D}_1 L(q, v) \tag{10b}$$
$$p = \mathrm{D}_2 L(q, v) \tag{10c}$$

This set of equations can be traced back to both, Lagrangian and Hamiltonian frameworks as it includes also the fibre derivative of the Legendre transformation (10c). Interestingly, the Lagrange multipliers p can be interpreted as conjugate momenta. It is worth noting that Hamiltonian and Lagrangian frameworks of mechanics are unified by Livens principle.

The novel GGL variational principle accounts for primary constraints (1) and secondary constraints (2). Similarly to the classical GGL stabilization (8), the GGL principle represents an index-reduction technique by minimal extension and yields DAEs with differentiation index $\nu_{\mathrm{d}} = 2$. In particular, the principle relies on the action integral

$$S_{\mathrm{GGL}}(q, v, p, \lambda, \gamma) = \int_0^T \left[L(q, v) - \lambda \cdot g(q) + p \cdot (\dot{q} - v - M^{-1}\,\mathrm{D}g(q)^{\mathrm{T}}\,\gamma)\right]\mathrm{d}t, \tag{11}$$

which generalizes Livens principle (9). Imposing the stationary condition $\delta S_{\mathrm{GGL}} = 0$, standard procedures of variational calculus and imposing endpoint conditions yields the Euler-Lagrange equations of the GGL principle as

$$\dot{q} = v + M^{-1}\mathrm{D}g(q)^{\mathrm{T}}\gamma, \tag{12a}$$
$$\dot{p} = \mathrm{D}_1 L(q, v) - \mathrm{D}g(q)^{\mathrm{T}}\lambda - \sum_{k=1}^{m} \gamma_k \mathrm{D}^2 g_k(q) M^{-1} p, \tag{12b}$$
$$p = \mathrm{D}_2 L(q, v), \tag{12c}$$
$$0 = g(q), \tag{12d}$$
$$0 = \mathrm{D}g(q)M^{-1}p. \tag{12e}$$

The above equations appear in a similar fashion as the classical GGL stabilization (8) with an additional term in (12b), which ensures the Hamiltonian structure of the equations. In particular, (12) can be written as

$$\dot{z} = \mathbb{J}\mathrm{D}H^{\lambda\gamma}_{\mathrm{GGL}}(z), \tag{13}$$

together with (12d) and (12e), yielding a similar Hamiltonian structure as in (7). The corresponding augmented Hamiltonian is given by $H^{\lambda\gamma}_{\mathrm{GGL}}(z) = H(q,p) + \lambda \cdot g(q) + \gamma \cdot G(q)M^{-1}p$. The above equations can be related to the Euler-Lagrange equations (12) of the GGL functional after elimination of the velocities by employing the Legendre transformation (12c). Similar to the classical GGL stabilization, the systems conservation properties (i.e. underlying structures) are not altered. Consequently, the Hamiltonian H itself, momentum maps J_ξ and the symplectic two-form ω are first integrals of solutions of (12). In contrast to the original GGL formulation, those conservation laws hold true regardless of the value of the Lagrange multipliers γ. The GGL principle can thus be seen as an ideal basis for the design of structure-preserving integrators.

3 Variational integrators (VI)

The concept of variational integrators relies on the direct approximation of the action integral instead of the corresponding equations of motion. The time interval $[0\ \ T]$ is subdivided into N timesteps of time step size h. The subintegrals are discretized with a discrete Lagrangian L_d, such that

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

The action integral is thus approximated by a discrete action sum S_d. Futhermore, the stationary condition

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

eventually yields the discrete Euler-Lagrange (DEL) equations, which determine the time-stepping scheme for the variational integrator. In Kinon & Betsch [1] a simple, first approach for discretizing the GGL principle (11) has been introduced. It is first order accurate, symplectic and conserves the systems momentum maps as well as primary constraints. However, secondary constraints are only satisfied in intermediate timesteps. We therefore now target the design of second order schemes and schemes, which also preserve velocity-level constraints exactly, while maintaining the same conservation properties. To this end, inspired by the one-stage theta method for optimally controlled systems by Betsch & Becker [5], we approximate the functional of the GGL principle by a discrete action sum given by

$$\begin{aligned} S^{\mathrm{d}}_{\mathrm{GGL}} = \sum_{n=0}^{N-1} \big[L^{\lambda}_{\mathrm{d}}(q^n, Q^n, v^{n+1}) + p^{n+1} \cdot \big(q^{n+1} - q^n - f^{\gamma}_{\mathrm{d}}(q^n, Q^n, v^{n+1})\big) \\ + P^n \cdot \big(Q^n \ \ - q^n - f^{\gamma}_{\mathrm{d}}(q^n, Q^n, v^{n+1})\big)\big], \end{aligned} \tag{14}$$

where auxiliary position vectors Q^n and momenta P^n are introduced. Moreover, in (14), L^{λ}_{d} represents a discrete version of the augmented Lagrangian for constrained mechanical systems such that

$$L^{\lambda}_{\mathrm{d}} \approx \int_{t^n}^{t^{n+1}} [L(q,v) - \lambda \cdot g(q)]\, \mathrm{d}t, \tag{15}$$

whereas f^{γ}_{d} denotes the discrete version of the right hand side vector of the kinematic equation (12a), such that $\dot{q} = f^{\gamma}(q,v)$. Discrete versions of the constraints, being enforced by Lagrange multiplier λ^n and γ^n, are part of the chosen L^{λ}_{d} and f^{γ}_{d}, respectively. Eventually, a whole family of variational integrators is generated. All members are symplectic by design and conserve the momentum maps associated with symmetries of the system. The corresponding DEL equations show that $Q^n = q^{n+1}$, such that auxiliary positions can be eliminated. Our approach evaluates the positions in an intermediate state, parameterized with $\alpha \in [0,1]$ such that

$$q^{n+\alpha} = (1-\alpha)\, q^n + \alpha\, q^{n+1}. \tag{16}$$

Moreover, the discrete Lagrangian shall be defined by

$$L^{\lambda}_{\mathrm{d}} = h\, L(q^{n+\alpha}, v^{n+1}) - \lambda^n \cdot g_{\mathrm{d}}(q^n, q^{n+1}), \tag{17}$$

where g_d is a discretization of the holonomic constraints (1) and f^{γ}_{d} is chosen as

$$f^{\gamma}_{\mathrm{d}}(q^n, q^{n+1}, v^{n+1}) = h\, v^{n+1} + h\, M^{-1} \mathrm{D}g(q^{n+\alpha})^{\mathrm{T}} \gamma^n. \tag{18}$$

One possible method generated by this approach is second order accurate but fullfils the constraints only in intermediate times ("VI-A"). It can be obtained by defining

$$g_{\mathrm{d}}^{\mathrm{A}}(q^n, q^{n+1}) = h\, g(q^{n+\alpha}). \tag{19}$$

Another option yields a first-order accurate scheme but satisfies both constraints exactly ("VI-B"). The corresponding discretization of the constraints makes use of an additional parameter $\theta \in [0, 1]$ such that

$$g_{\mathrm{d}}^{\mathrm{B}}(q^n, q^{n+1}) = h\, \left[(1-\theta) g(q^n) + \theta g(q^{n+1})\right]. \tag{20}$$

Consequently, both drawbacks of the first approach proposed in Kinon & Betsch [1] have been prevented by this novel ansatz (14), which represents a versatile discretization method for the structure-preserving integration of constrained dynamical systems. Further details on the resulting integration schemes can be found in [8].

4 Energy-Momentum scheme

Another class of structure-preserving integrators is given by so-called energy-momentum schemes (EMS). Assuming a constrained Hamiltonian system with symmetries, the Hamiltonian equations of motion of the GGL functional (13), (12d) and (12e) can be discretized as

$$z^{n+1} - z^n = h\, \bar{D}^{\mathrm{G}} H_{\mathrm{GGL}}^{\lambda\gamma}(z^n, z^{n+1}), \tag{21a}$$

$$g^q(q^{n+1}) = 0, \tag{21b}$$

$$g^v(z^{n+1}) = 0, \tag{21c}$$

for $n = 0, ..., N-1$. Note that the G-equivariant discrete derivative $\bar{D}^{\mathrm{G}}$ by Gonzalez [6] has been used. The Gonzalez discrete gradient of a function $f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is defined as

$$\bar{D} f(x, y) = \mathrm{D} f(z) + \frac{f(y) - f(x) - \mathrm{D} f(z) \cdot (y - x)}{||y - x||} (y - x) \tag{22}$$

with $z = \frac{1}{2}(x + y)$. It satisfies the crucial *directionality condition*

$$\bar{D} f(x, y) \cdot (y - x) = f(y) - f(x), \tag{23}$$

which ensures the conservation properties of energy-momentum schemes. The G-equivariant formulation assumes r, at most quadratic invariants $\pi_i \in \mathbb{R}$ of f such that

$$\bar{D}^{\mathrm{G}} f(x, y) = \sum_{i=1}^{r} \mathrm{D}\pi_i(z) \cdot \bar{D} \tilde{f}(\pi_i(x), \pi_i(y)), \tag{24}$$

where $f(x, y) = \tilde{f}(\{\pi_i\}_{i=1}^r)$. Eventually, the time-stepping scheme (21) generalizes the method proposed by Gonzalez [6] with respect to velocity level constraints $g^v(z)$. As the name suggests, this scheme conserves the Hamiltonian and the momentum maps exactly and is second-order accurate as the discrete gradient enhances the standard gradient evaluated in the midpoint. We refer to [8] for further details on the resulting EMS.

5 Numerical results

We simulate the four-particle system from Gonzalez [6] with $h = 0.05$ and a total simulation time of $T = 10$. The system consists of four masses m_i, which are subject to the initial conditions $q_1^0 = (0, 0, 0)^{\mathrm{T}}$, $q_2^0 = (1, 0, 0)^{\mathrm{T}}$, $q_3^0 = (0, 1, 0)^{\mathrm{T}}$ and $q_4^0 = (1, 1, 0)^{\mathrm{T}}$. The masses are interconnected by two rigid bars, which impose primary constraints

$$g_1(q) = \frac{1}{2}\left[\frac{1}{l_{12}^2}(q_2 - q_1) \cdot (q_2 - q_1) - 1\right], \tag{25a}$$

$$g_1(q) = \frac{1}{2}\left[\frac{1}{l_{34}^2}(q_4 - q_3) \cdot (q_4 - q_3) - 1\right] \tag{25b}$$

and two spring elements k_i, which give rise to the system's potential function

$$V = \frac{1}{2} k_1 \left((q_3 - q_1) \cdot (q_3 - q_1) - l_{13}^2\right)^2 + \frac{1}{2} k_2 \left((q_4 - q_2) \cdot (q_4 - q_2) - l_{24}^2\right)^2. \tag{26}$$

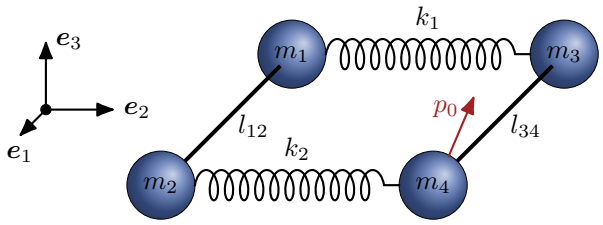

Fig. 1: Four-particle system

Table 1: Parameters

m_i	$\{1,\ 3,\ 2.3,\ 1.7\}$	kg
k_i	$\{1,\ 10\}$	N/m
l_{ij}	1	m
p_0	$(0, 3, 2)^{\mathrm{T}}$	kg m/s

The bars have lengths l_{12} and l_{34} and the springs' natural lengths are denoted by l_{13} and l_{24}. At $t = 0$ an initial momentum p_0 is imposed on the fourth mass. We want to compare the abovementioned schemes as well as the classical GGL stabilization (8) discretised by the midpoint rule ("GGL-MP") with endpoint evaluation of the constraints. The computations have been performed using *metis*, which is freely available at [7]. The parameter values are comprised in Table 1.

The VI-B method and the EMS as well as the classical GGL method preserve both primary and secondary constraints (up to numerical round-off), whereas the VI-A does not (compare Fig. 2). However, when it comes to the preservation of momentum, we can observe, that all schemes, which have been developed by using the GGL principle outperform the classical GGL scheme (see Fig. 3). Furthermore, it can be seen that the EMS additionally preserves the system's Hamiltonian (cf. Fig. 3). The results validate the previous findings and underline the beneficial structure of the GGL principle for the design of structure-preserving integrators.

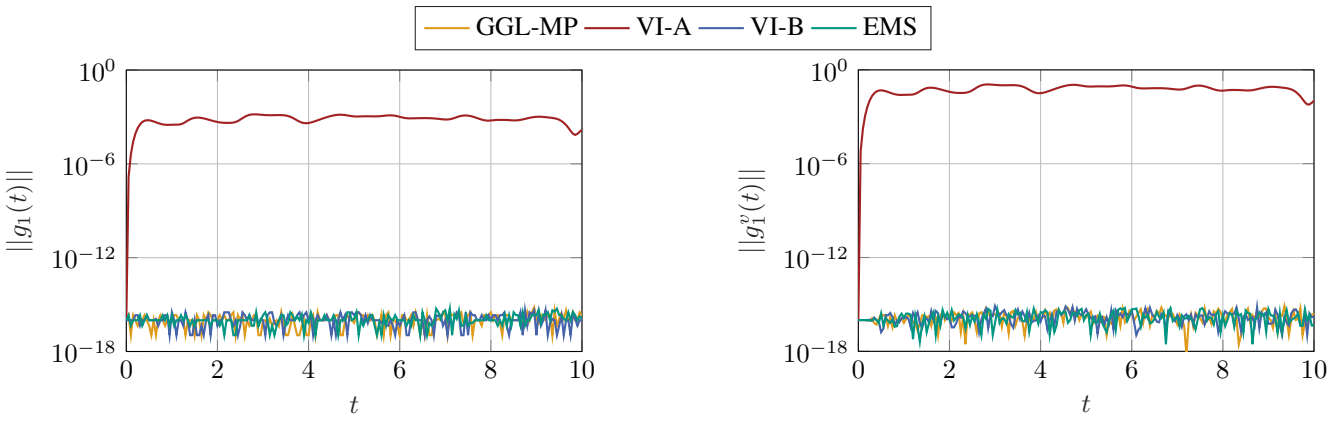

Fig. 2: Conservation of primary (left) and secondary constraints (right)

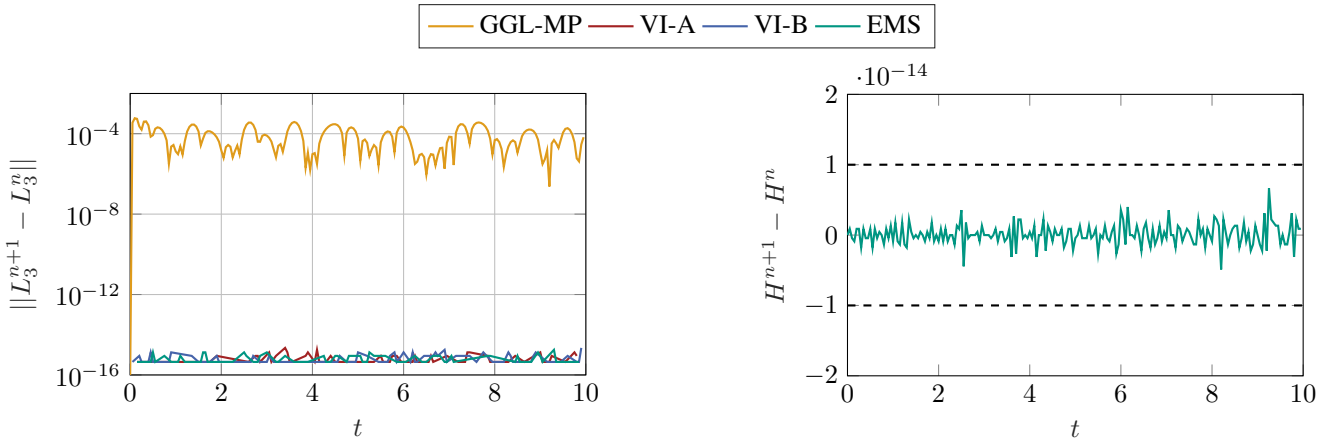

Fig. 3: Conservation of angular momentum about 3-axis (left) and Hamiltonian (right)

6 Conclusion

In this work, we have taken up the recently introduced GGL variational principle (cf. Kinon & Betsch [1]). It extends Livens principle by accounting for both primary and secondary constraints. Due to its mixed nature, it unifies Lagrangian and Hamiltonian frameworks. The GGL principle enhances the well-known Gear-Gupta-Leimkuhler stabilization and consequently achieves and index reduction to $\nu_{\mathrm{d}} = 2$ to avoid numerical instabilities. Contrary to the original formulation, the equations of motion have Hamiltonian structure, which facilitates the design of structure-preserving integrators, as crucial conservation properties do not depend on the value of the Lagrange multipliers. Furthermore, two classes of structure-preserving time-stepping schemes for constrained mechanical systems have been introduced: a family of variational integrators and an energy-momentum scheme. Both are capable of conserving the system's momentum maps and tackle the problem of drift adequately. For further analyses, details and proofs concerning the presented methods we refer to [8].

In the future, for the search of further structure-preserving integrators based on the GGL functional, one might focus on the construction of higher order methods. Therefore, two different approaches are promising: Firstly, partioned Runge Kutta schemes that can be gained as variational integrators from Livens principle could be generalized with respect to constrained dynamics. The work by Bou-Rabee [9] might serve as a starting point. Secondly, one might aim for Galerkin-based methods for constrained systems corresponding to an already existing work by Ober-Blöbaum [10]. Another promising idea is the application of continuous Galerkin schemes for index 2 DAEs to the novel functional for constrained dynamics. Altmann & Herzog [11] have recently provided a corresponding framework.

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