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Order reduction in time integration caused by velocity projection[§]

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ABSTRACT

Holonomic constraints restrict the configuration of a multibody system to a subset of the configuration space. They imply so called hidden constraints at the level of velocity coordinates that may formally be obtained from time derivatives of the original holonomic constraints. A numerical solution that satisfies hidden constraints as well as the original constraint equations may be obtained considering both types of constraints simultaneously in each time step (*stabilized index-2 formulation*) or using *projection* techniques. Both approaches are well established in the time integration of differential-algebraic equations. Recently, we have introduced a generalized-α Lie group time integration method for the stabilized index-2 formulation that achieves second order convergence for all solution components. In the present paper, we show that a separate velocity projection would be less favourable since it may result in an order reduction and in large transient errors after each projection step. This undesired numerical behaviour is analysed by a one-step error recursion that considers the coupled error propagation in differential and algebraic solution components. This one-step error recursion has been used before to prove second order convergence for the application of generalized-α methods to constrained systems. As a technical detail, we discuss the extension of these results from symmetric, positive definite mass matrices to the rank deficient case.

1 INTRODUCTION

Backward differentiation formulae (BDF) and Newmark type methods are the most popular classes of time integration methods in industrial multibody system simulation [4, 17]. They do not share the favourable nonlinear stability properties of variational integrators and structure-preserving integrators in the long-term integration of conservative systems but prove to be very efficient in the application to multibody system models with dissipative terms resulting, e.g., from friction forces or control structures. BDF gain much efficiency from a variable step size, variable order implementation that allows to adapt time step size and order to the solution behaviour [6]. In the application to flexible multibody systems with nonlinear flexible components, the large amount of algorithmic damping may be considered as a potential drawback of BDF methods since all higher frequency solution components are strongly damped in the step size range of practical interest.

For this problem class, Newmark type methods like the generalized-α method of Chung and Hulbert [11] offer more flexibility since the damping properties for high frequency modes in linear systems may be controlled by appropriate algorithmic parameters. For these methods, the order of convergence is limited to two but in a method of lines framework this order barrier does typically not result in strong limitations of the time step size since the error of space discretization has to be considered anyway. For constrained systems, the direct application of Newmark type methods to the constrained equations of motion proves to be quite popular because of its straightforward implementation in existing large scale simulation tools [10, 17, 22], see also [5]. Index reduction techniques [6, 13, 16] that are a quasi-standard for BDF solvers in industrial multibody system simulation [4] have been proposed as well for Newmark type methods [20, 21], see also [3], but implementations without index reduction still dominate in industrial simulation tools [17, 22].

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An extension of generalized-α methods to mechanical systems that have a configuration space with Lie group structure has been proposed in [8]. It relies again on the direct time discretization of the constrained equations of motion. On the Lie group, these constrained systems form a differential-algebraic equation (DAE) that may be studied analytically by an extension of classical DAE theory [6, 19]. Holonomic constraints result in a Lie group DAE of index three. As in classical DAE theory, they imply (hidden) constraints at the level of velocity coordinates that are obtained by differentiation w.r.t. time t, see [6, 13].

Inspired by numerically observed large transient errors and spurious oscillations of the constraint forces in the Lie group time integration of a heavy top benchmark problem [7], we have studied the error propagation in generalized-α methods for index-3 DAEs on Lie groups in great detail [2, 3, 9]. A one-step error recursion for the algebraic solution components shows that starting values being consistent with the hidden constraints at velocity level may result in order reduction and in a large oscillating first order error term that is damped out rapidly after a short transient phase. These numerical problems could be avoided by perturbed starting values or by the simultaneous consideration of original and hidden constraints in the stabilized index-2 formulation of the equations of motion [3].

In the present paper, we recall basic aspects of the generalized-α Lie group method (Section 2) and use recently obtained convergence results to study the influence of velocity projections on the accuracy of the numerical solution (Section 3). In contrast to known error estimates for projection techniques in DAE time integration [12, 19], we observe an order reduction if the direct time discretization of the index-3 DAE is combined with separate projection steps to get a numerical solution that satisfies the hidden constraints at velocity level. The extension of this error analysis to multibody system models with rank deficient mass matrix is discussed in Section 4.

2 THE GENERALIZED-α LIE GROUP TIME INTEGRATION METHOD

In the Lie group setting, the configuration space G of a multibody system forms a k-dimensional manifold with Lie group structure. For a constrained system with mass matrix $\mathbf{M}$ and force vector $\mathbf{g}$, the generalized coordinates $q \in G$ are solutions of the Lie group DAE

$$
\begin{aligned}
\dot{q} &= DL_q(e) \cdot \widetilde{\mathbf{v}}\,, && \text{(1a)}\\
\mathbf{M}(q)\dot{\mathbf{v}} &= -\mathbf{g}(q,\mathbf{v},t) - \mathbf{B}^\top(q)\boldsymbol{\lambda}\,, && \text{(1b)}\\
\boldsymbol{\Phi}(q) &= \mathbf{0} && \text{(1c)}
\end{aligned}
$$

with the velocity vector $\mathbf{v} \in \mathbb{R}^k$ and an invertible linear mapping $\widetilde{(\bullet)} : \mathbb{R}^k \to T_eG,\ \mathbf{v} \mapsto \widetilde{\mathbf{v}}$. Here, $e \in G$ is the identity element and T_qG denotes the tangent space of G at point $q \in G$, see [8, 9] for a more detailed discussion. The tangent space $T_eG =: \mathfrak{g}$ is also known as the Lie algebra corresponding to Lie group G. It is mapped bijectively to T_qG by the directional derivative $DL_q(e)$ of the left translation map $L_q : G \to G,\ y \mapsto q \circ y$ evaluated at e. Here, symbol "$\circ$" stands for the group operation in G.

The m holonomic constraints (1c) are coupled to the dynamical equations (1b) by Lagrange multipliers $\boldsymbol{\lambda}(t) \in \mathbb{R}^m$ and by the matrix $\mathbf{B}(q) \in \mathbb{R}^{m\times k}$ that represents the constraint gradients in the sense that

$$
D\boldsymbol{\Phi}(q) \cdot \big(DL_q(e) \cdot \widetilde{\mathbf{w}}\big) = \mathbf{B}(q)\mathbf{w}\,, \quad (\,\mathbf{w} \in \mathbb{R}^k\,) \tag{2}
$$

with $D\boldsymbol{\Phi}(q) \cdot \big(DL_q(e) \cdot \widetilde{\mathbf{w}}\big)$ denoting the directional derivative of $\boldsymbol{\Phi} : G \to \mathbb{R}^m$ evaluated at $q \in G$ in the direction $DL_q(e) \cdot \widetilde{\mathbf{w}} \in T_qG$. It is assumed that $\mathbf{B}(q)$ has full rank $m \le k$ and that the mass matrix $\mathbf{M}(q)$ is symmetric, positive definite. Systems with rank deficient mass matrix are considered in Section 4 below. For simplicity, we restrict ourselves to scleronomic constraints (1c) throughout the present paper. All results remain, however, valid as well in the case of rheonomic constraints $\boldsymbol{\Phi}(q,t) = \mathbf{0}$ that depend explicitly on time t.

Readers who are not familiar with the Lie group setting might for the moment abstract from many technical details considering the special case of a linear configuration space $G = \mathbb{R}^k$ with vector valued elements $\mathbf{q} \in \mathbb{R}^k$ that will be denoted by boldface letters throughout this presentation. In linear spaces, the kinematic relations (1a) are simplified to $\dot{\mathbf{q}} = \mathbf{v}$ and the constraint matrix $\mathbf{B}(\mathbf{q})$ is given by the Jacobian $(\partial\boldsymbol{\Phi}/\partial\mathbf{q})(\mathbf{q})$.

The most straightforward approach to the time integration of constrained systems relies on a direct time discretization of the equations of motion in their original form (1). In linear spaces, the discretization of the kinematic equations (1a) is based on the Taylor expansion $\mathbf{q}(t+h) = \mathbf{q}(t) + h\mathbf{v}(t) + \frac{h^2}{2}\dot{\mathbf{v}}(t) + \mathcal{O}(h^3)$, ($h \to 0$), that is in the Lie group setting generalized to

$$q(t+h) = q(t) \circ \exp\big(h\widetilde{\mathbf{v}}(t) + \frac{h^2}{2}\widetilde{\dot{\mathbf{v}}}(t) + \mathcal{O}(h^3)\big)\,, \quad (\,h \to 0\,)$$

with the exponential map $\exp\,:\,\mathfrak{g} \to G$. For matrix Lie groups G, this exponential map is formally given by its series expansion $\exp(\widetilde{\mathbf{w}}) = \sum_i \widetilde{\mathbf{w}}^i/i!$. As proposed in [8], we consider a generalized-α Lie group method that updates the numerical solution $(q_n, \mathbf{v}_n, \mathbf{a}_n, \boldsymbol{\lambda}_n)$ in time step $t_n \to t_n + h$ according to

$$q_{n+1} = q_n \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}_n})\,, \tag{3a}$$
$$\boldsymbol{\Delta}\mathbf{q}_n = \mathbf{v}_n + (0.5-\beta)h\mathbf{a}_n + \beta h\mathbf{a}_{n+1}\,, \tag{3b}$$
$$\mathbf{v}_{n+1} = \mathbf{v}_n + (1-\gamma)h\mathbf{a}_n + \gamma h\mathbf{a}_{n+1}\,, \tag{3c}$$
$$(1-\alpha_m)\mathbf{a}_{n+1} + \alpha_m\mathbf{a}_n = (1-\alpha_f)\dot{\mathbf{v}}_{n+1} + \alpha_f\dot{\mathbf{v}}_n \tag{3d}$$

with vectors $\dot{\mathbf{v}}_{n+1}$, $\boldsymbol{\lambda}_{n+1}$ satisfying the equilibrium conditions

$$\mathbf{M}(q_{n+1})\dot{\mathbf{v}}_{n+1} = -\mathbf{g}(q_{n+1}, \mathbf{v}_{n+1}, t_{n+1}) - \mathbf{B}^\top(q_{n+1})\boldsymbol{\lambda}_{n+1}\,, \tag{3e}$$
$$\boldsymbol{\Phi}(q_{n+1}) = \mathbf{0}\,. \tag{3f}$$

In linear spaces, the update formula (3a) for the position coordinates is simplified to $\mathbf{q}_{n+1} = \mathbf{q}_n + h\boldsymbol{\Delta}\mathbf{q}_n$. Method (3) is characterized by algorithmic parameters α_m, α_f, β and γ that are typically selected based on the linear stability analysis for generalized-α methods in linear spaces according to Chung and Hulbert [11]. Throughout the paper, we suppose that the order condition $\gamma = 1/2 - \Delta_\alpha$ with $\Delta_\alpha := \alpha_m - \alpha_f$ is satisfied to guarantee a local truncation error of size $\mathcal{O}(h^3)$ for unconstrained systems in linear spaces.

3 ORDER REDUCTION CAUSED BY VELOCITY PROJECTION

In the 1990's, the DAE aspects of constrained systems (1) in linear spaces were studied in great detail, see, e.g., [19] for a compact summary. Generalizing these classical results to the Lie group setting in (1), we get *hidden* constraints at the level of velocity coordinates differentiating (1c) w.r.t. t:

$$\mathbf{0} = \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Phi}(q(t)) = D\boldsymbol{\Phi}(q(t))\cdot\dot{q}(t) = D\boldsymbol{\Phi}(q)\cdot\big(DL_q(e)\cdot\widetilde{\mathbf{v}}\big) = \mathbf{B}(q)\mathbf{v}\,, \tag{4}$$

see (2). For a second differentiation step that results in hidden constraints

$$\mathbf{0} = \frac{\mathrm{d}}{\mathrm{d}t}\big(\mathbf{B}(q(t))\mathbf{v}(t)\big) = \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Theta}\big(q(t), \mathbf{v}(t)\big) = \mathbf{B}(q)\dot{\mathbf{v}} + \mathbf{Z}(q)\big(\mathbf{v}, \mathbf{v}\big)\,. \tag{5}$$

at the level of acceleration coordinates, we consider the directional partial derivative of function $\boldsymbol{\Theta}(q, \mathbf{z}) := \mathbf{B}(q)\mathbf{z}$ w.r.t. $q \in G$ that may be represented by a bilinear form $\mathbf{Z}(q)\,:\,\mathbb{R}^k \times \mathbb{R}^k \to \mathbb{R}^m$ with

$$D_q\boldsymbol{\Theta}(q, \mathbf{z})\cdot\big(DL_q(e)\cdot\widetilde{\mathbf{w}}\big) = \mathbf{Z}(q)(\mathbf{z}, \mathbf{w})\,, \quad (\,\mathbf{z}, \mathbf{w} \in \mathbb{R}^k\,)\,,$$

see [3]. In linear spaces, $\mathbf{Z}(q)$ is given by the curvature terms $(\partial^2\boldsymbol{\Phi}/\partial\mathbf{q}^2)(\mathbf{q})$.

The generalized-α time integration method (3) discretizes the equations of motion (1) directly, i.e., without considering any hidden constraints. An alternative to this approach are DAE time integration methods that are based on index reduction before time discretization and use hidden constraints like (4) and (5). If the original constraints (1c) are simply substituted by (4) or by (5), we get the index-2 formulation or the index-1 formulation of the equations of motion [19]. In contrast to the numerical solution q_{n+1} in the generalized-α method (3) that remains for all time steps $t_n \to t_{n+1} = t_n + h$ in the constraint manifold $\mathfrak{M} := \{\, q \in G\,:\,\boldsymbol{\Phi}(q) = \mathbf{0}\,\}$, see (3f), there is no guarantee that the holonomic constraints (1c) are exactly satisfied by numerical solutions q_{n+1} for index reduced formulations. We observe a linear (index-2 formulation) or quadratic (index-1 formulation) *drift-off effect*, i.e., $\|\boldsymbol{\Phi}(q_n)\|$ grows like $c_2(t_n - t_0)$ or like $c_1(t_n - t_0)^2$, respectively.

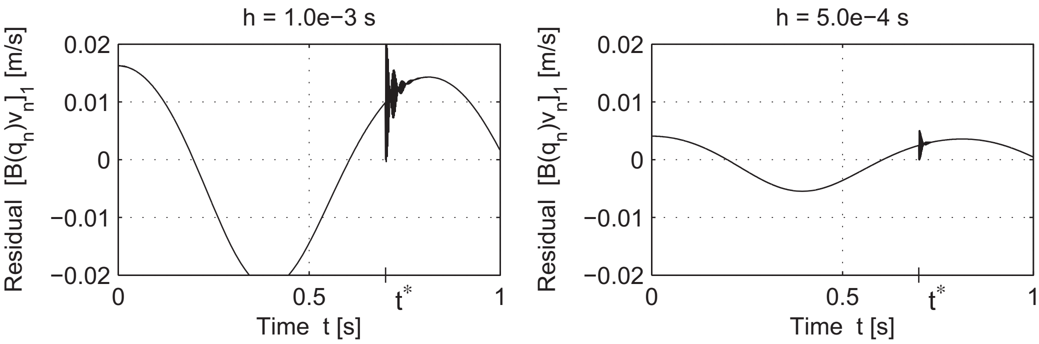

Figure 1: Heavy top benchmark [9, 17], generalized-α method (3) with $h = 1.0 \times 10^{-3}$ s (left plot) and $h = 5.0 \times 10^{-4}$ s (right plot): First component of the residual in hidden constraints (4). Velocity projection at $t = t^* = 0.7\,$s.

To avoid this constraint violation in index reduced formulations, the numerical solution q_{n+1} is projected onto $\mathfrak{M}$ before continuing time integration with the next time step $t_{n+1} \to t_{n+2}$, see [12, 19]. In the Lie group setting, the classical projection step $\mathbf{q}_{n+1} \to \mathbf{q}_{n+1} + \mathbf{dq}_{n+1}$ with $\mathbf{dq}_{n+1} \in \mathbb{R}^k$ denoting the solution of the constrained minimization problem $\min \{\, \|\mathbf{dq}\| \,:\, \mathbf{\Phi}(\mathbf{q}_{n+1} + \mathbf{dq}) = \mathbf{0} \,\}$ may be generalized to

$$q_{n+1} \mapsto q_{n+1} \circ \exp(\widetilde{\mathbf{dq}}_{n+1}) \;\text{ with }\; \mathbf{dq}_{n+1} := \text{argmin} \{\, \|\mathbf{dq}\| \,:\, \mathbf{\Phi}\big(q_{n+1} \circ \exp(\widetilde{\mathbf{dq}})\big) = \mathbf{0} \,\}\,, \tag{6}$$

see also the work of Terze et al. [23] on projection techniques in the Lie group context. The velocity vector $\mathbf{v}_{n+1}$ should be projected to the tangential space $T_q\mathfrak{M}$ at $q = q_{n+1} \circ \exp(\widetilde{\mathbf{dq}}_{n+1})$, see (6), by

$$\mathbf{v}_{n+1} \mapsto \mathbf{v}_{n+1} + \mathbf{dv}_{n+1} \;\text{ with }\; \mathbf{dv}_{n+1} := \text{argmin} \{\, \|\mathbf{dv}\| \,:\, \mathbf{B}(q)(\mathbf{v}_{n+1} + \mathbf{dv}) = \mathbf{0} \,\}\,. \tag{7}$$

The combination of index reduction and projection techniques is well established in DAE time integration of higher index systems [19]. The extra errors being introduced by the projection of q_{n+1}, $\mathbf{v}_{n+1}$ to $\mathfrak{M}$ and $T_q\mathfrak{M}$ according to (6) and (7) remain in the size of discretization errors and do not deteriorate the order of convergence. This result follows from the observation that $q(t) \in \mathfrak{M}$ and $\mathbf{v}(t) \in T_{q(t)}\mathfrak{M}$, ($t \geq t_0$), such that after one time step the numerical solution q_{n+1}, $\mathbf{v}_{n+1}$ of a method with local error $\mathcal{O}(h^{p+1})$ is always $\mathcal{O}(h^{p+1})$-close to the manifold and to its tangential space. Therefore, the increments $\mathbf{dq}_{n+1}$, $\mathbf{dv}_{n+1}$ in the projection steps (6) and (7) remain in the size of the local error $\mathcal{O}(h^{p+1})$, see [19, Section VII.2].

The drift-off effect is typical of index reduced formulations and does not affect the generalized-α method (3) that discretizes the original Lie group index-3 DAE directly resulting in $\mathbf{\Phi}(q_{n+1}) = \mathbf{0}$, see (3f). In the hidden constraints at velocity level, we observe a residual of size $\|\mathbf{B}(q_{n+1})\mathbf{v}_{n+1}\| = \mathcal{O}(h^2)$ that corresponds to the global error of order two for the numerical solution q_{n+1}, $\mathbf{v}_{n+1}$. To illustrate this numerical effect, we apply (3) with algorithmic parameters according to [11] and a damping ratio at infinity of $\rho_\infty = 0.9$ to the heavy top benchmark problem [8, 9, 17]. The equations of motion and all model parameters are given in the appendix below. The equations are formulated in the Lie group $\mathbb{R}^3 \times \mathrm{SO}(3)$ with $m = 3$ holonomic constraints that result in 3 hidden constraints at velocity level. Fig. 1 shows one component of the constraint residual $\mathbf{B}(q)\mathbf{v}$ vs. t for time step sizes $h = h_0 = 10^{-3}$ s (left plot) and $h = h_0/2$ (right plot). Up to a discontinuity at $t^* = 0.7\,$s (that will be discussed in more detail below) the constraint residual oscillates smoothly with an amplitude that is decreased by a factor of $2^2 = 4$ if the step size is reduced by a factor of 2.

Despite these rather large residuals in the hidden constraints (4), the generalized-α method (3) with reasonable starting values [3] converges with order $p = 2$ in all solution components. For the Lagrange multipliers $\boldsymbol{\lambda}$, this is illustrated by the dashed line in the right plot of Fig. 2 that has slope $+2$ in double logarithmic scale. After impacts in the mechanical system and after step size changes it would, however, be quite natural to enforce zero constraint residuals (4) by a projection of $\mathbf{v}_{n+1}$ to the tangential space $T_{q_{n+1}}\mathfrak{M}$ according to (7) with $\|\mathbf{dv}\| := (\mathbf{dv}^\top \mathbf{M}(q)\mathbf{dv})^{1/2}$ and $q = q_{n+1}$, i.e., we substitute $\mathbf{v}_{n+1}$ at $t = t_{n+1}$ by its projection

$$\mathbf{v}^*_{n+1} := \big(\mathbf{I}_k - [\mathbf{M}^{-1}\mathbf{B}^\top(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top)^{-1}\mathbf{B}](q_{n+1})\big)\mathbf{v}_{n+1}$$

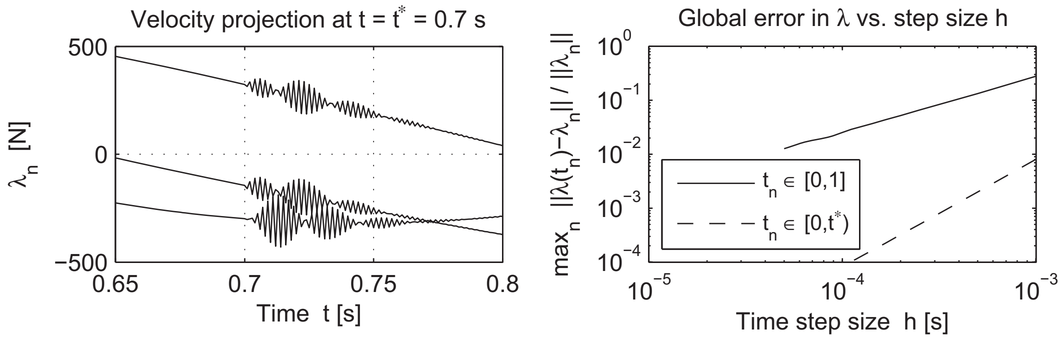

Figure 2: Heavy top benchmark [9, 17], generalized-α method (3), Velocity projection at $t = t^* = 0.7\,\mathrm{s}$. Left plot: Numerical solution λ_n for $h = 1.0 \times 10^{-3}\,\mathrm{s}$, $t \in [0.65\,\mathrm{s}, 0.8\,\mathrm{s}]$, Right plot: Maximum of the norm of global errors in λ in a time interval that contains t^* (solid line) and in the subinterval $[0, t^*)$ (dashed line).

onto the tangential space $T_q\mathfrak{M}$ at $q = q_{n+1}$, see also [15, 19] for a more detailed discussion of velocity projection in DAE time integration.

Taking into account the positive convergence results for the combination of index reduction and projection techniques that were discussed above, we might expect that such a velocity projection does also not deteriorate the second order convergence of the generalized-α method (3).

The test results in Fig. 1 and in the left plot of Fig. 2 show, however, that a velocity projection at $t_{n^*} = t^* = 0.7\,\mathrm{s}$ results in oscillating constraint residuals and in spurious oscillations of large amplitude in the numerical solution $\boldsymbol{\lambda}_n$ that are damped out after about 100 time steps. Furthermore, we observe an order reduction for the Langrange multipliers $\boldsymbol{\lambda}$ that is illustrated by a solid line of slope $+1$ in the right plot of Fig. 2. This plot shows in terms of relative errors $\|\boldsymbol{\lambda}(t_n) - \boldsymbol{\lambda}_n\|/\|\boldsymbol{\lambda}_n\|$ the maximum of the norm of global errors in components $\boldsymbol{\lambda}$ for $t < t^*$ (i.e., without velocity projection, dashed line) and for $t \in [0, 1]$ (i.e., with velocity projection at $t = t^*$, solid line). The maximum of global errors in $[0, 1]$ is dominated by the large error terms in the transient phase after the velocity projection at $t = t^*$.

The undesired numerical results reflect a coupled one-step recursion for the scaled constraint residuals $\mathbf{B}(q_n)\mathbf{v}_n/h$ and the global errors in components $\boldsymbol{\lambda}$ and $\mathbf{B}(q)\mathbf{a}$ that is given by

$$\mathbf{E}_{n+1} = \big((\mathbf{T}_+^{-1}\mathbf{T}_0) \otimes \mathbf{I}_m\big)\mathbf{E}_n + \mathcal{O}(h^2) \;\text{ with }\; \mathbf{E}_n := \begin{pmatrix} \frac{1}{h}\mathbf{B}(q_n)\mathbf{v}_n + h\mathbf{B}\big(q(t_n)\big)\mathbf{r}(t_n) + \boldsymbol{\zeta}_n \\ [\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top]\big(q(t_n)\big)\big(\boldsymbol{\lambda}(t_n) - \boldsymbol{\lambda}_n\big) \\ \mathbf{B}\big(q(t_n)\big)\big(\dot{\mathbf{v}}(t_n + \Delta_\alpha h) - \mathbf{a}_n\big) \end{pmatrix} \tag{8}$$

with $\widetilde{\mathbf{r}}(t) = \big(2(1 - 6\beta - 3\Delta_\alpha)\ddot{\widetilde{\mathbf{v}}}(t) + \widetilde{\mathbf{v}}(t)\dot{\widetilde{\mathbf{v}}}(t) - \dot{\widetilde{\mathbf{v}}}(t)\widetilde{\mathbf{v}}(t)\big)/12$ and a vector $\boldsymbol{\zeta}_n = \mathcal{O}(h^2)$ that depends in a complicated way on the global error in the position coordinates q and vanishes on initialization [3]. The Kronecker product $(\mathbf{T}_+^{-1}\mathbf{T}_0) \otimes \mathbf{I}_m$ is composed of matrices

$$\mathbf{T}_+ := \begin{pmatrix} 0 & 0 & -\beta \\ 1 & 0 & -\gamma \\ 0 & 1-\alpha_f & 1-\alpha_m \end{pmatrix}, \quad \mathbf{T}_0 := \begin{pmatrix} 1 & 0 & 0.5-\beta \\ 1 & 0 & 1-\gamma \\ 0 & -\alpha_f & -\alpha_m \end{pmatrix}$$

and the identity matrix $\mathbf{I}_m$. For algorithmic parameters α_m, α_f, β and γ according to Chung and Hulbert [11], the spectral radius of the iteration matrix in (8) is given by $\varrho(\mathbf{T}_+^{-1}\mathbf{T}_0) = \rho_\infty$ with $\rho_\infty \in [0, 1]$ denoting the damping ratio at infinity.

Without any projection steps, the constraint residuals $\mathbf{B}(q_n)\mathbf{v}_n$ for the generalized-α method (3) are of size $\mathcal{O}(h^2)$, see Fig. 1. The scaled constraint residuals $\mathbf{B}(q_n)\mathbf{v}_n/h$ in the first component of $\mathbf{E}_n$ compensate the first order error term $h\mathbf{B}(q(t))\mathbf{r}(t)$, see (8), and result in $\mathbf{E}_n = \mathcal{O}(h^2)$ if $\rho_\infty < 1$ and the starting values $\mathbf{v}_0$, $\mathbf{a}_0$ are defined such that $\mathbf{E}_0 = \mathcal{O}(h^2)$, see [3].

The velocity projection at $t^* = t_{n^*} = 0.7\,\mathrm{s}$ eliminates the constraint residual $\mathbf{B}(q_n)\mathbf{v}_n$ at $n = n^*$. Therefore, the compensation of term $h\mathbf{B}(q(t^*))\mathbf{r}(t^*)$ in the first component of $\mathbf{E}_{n^*}$ is now missing and we get an additional first order error term $\big((\mathbf{T}_+^{-1}\mathbf{T}_0)^{n-n^*}\otimes\mathbf{I}_m\big)\mathbf{E}_{n^*}$ for all $n\geq n^*$ that results in order reduction for components $\boldsymbol{\lambda}$. Analysing $\|(\mathbf{T}_+^{-1}\mathbf{T}_0)^{\bar{n}}\|$ by a transformation to Jordan canonical form, see [3], we get the error bound $\|\boldsymbol{\lambda}(t_n)-\boldsymbol{\lambda}_n\|\leq C\big(\bar{n}^2\rho_\infty^{\bar{n}}h+h^2\big)$ with $\bar{n}:=n-n^*\geq 0$ and a suitable constant $C>0$.

4 RANK DEFICIENT MASS MATRICES

To prove the convergence of generalized-α methods in the constrained case, we studied the coupled error propagation in differential and algebraic solution components and supposed that the symmetric mass matrix $\mathbf{M}(q)\in\mathbb{R}^{k\times k}$ is positive definite and the constraint Jacobian $\mathbf{B}(q)\in\mathbb{R}^{m\times k}$ with $m\leq k$ has full rank along the solution [1, 3, 9]. With these assumptions, the dynamical equations in (1) and the hidden constraints (5) at the level of acceleration coordinates may be summarized in a system of $k+m$ linear equations

$$\begin{pmatrix}\mathbf{M}(q) & \mathbf{B}^\top(q)\\ \mathbf{B}(q) & \mathbf{0}\end{pmatrix}\begin{pmatrix}\dot{\mathbf{v}}\\ \boldsymbol{\lambda}\end{pmatrix}=\begin{pmatrix}-\mathbf{g}(q,\mathbf{v},t)\\ -\mathbf{Z}(q)\big(\mathbf{v},\mathbf{v}\big)\end{pmatrix} \tag{9}$$

that is solved straightforwardly:

$$\dot{\mathbf{v}} = -\big(\mathbf{I}-\mathbf{M}^{-1}\mathbf{B}^\top(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top)^{-1}\mathbf{B}\big)\mathbf{M}^{-1}\mathbf{g}-\mathbf{M}^{-1}\mathbf{B}^\top(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top)^{-1}\mathbf{Z}\,, \tag{10a}$$

$$\boldsymbol{\lambda} = -(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top)^{-1}\mathbf{B}\mathbf{M}^{-1}\mathbf{g}+(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top)^{-1}\mathbf{Z}\,. \tag{10b}$$

The formal differentiation of (10b) w.r.t. t yields $\dot{\boldsymbol{\lambda}}=\dot{\boldsymbol{\lambda}}(q,\mathbf{v},t)$ and proves that (1) forms an index-3 DAE, see, e.g., the corresponding index analysis for the equations of motion in linear spaces in [19].

This index analysis may be generalized to a certain class of constrained systems (1) with rank deficient, i.e. singular mass matrix $\mathbf{M}(q)$, see [14, 17]. Following the presentation in [17, Section 10.2], we multiply the second block row of (9) by $\mathbf{B}^\top(q)$ and add the resulting equation to the first block row to get an equivalent system (9) with $\mathbf{M}$, $\mathbf{g}$ being substituted by

$$\mathbf{M}^*:=\mathbf{M}+\mathbf{B}^\top\mathbf{B}\,,\;\; \mathbf{g}^*:=\mathbf{g}+\mathbf{B}^\top\mathbf{Z}\,.$$

For symmetric, positive semi-definite mass matrices $\mathbf{M}(q)$, matrix $\mathbf{M}^*(q)$ is positive definite (and therefore also non-singular) if and only if $\mathbf{M}(q)$ is positive definite at the null space of $\mathbf{B}(q)$ since the two conditions $\boldsymbol{\xi}^\top\mathbf{M}\boldsymbol{\xi}\geq 0$, ($\boldsymbol{\xi}\in\mathbb{R}^k$), and $\boldsymbol{\xi}^\top\mathbf{M}\boldsymbol{\xi}>0$, ($\boldsymbol{\xi}\in\mathbb{R}^k\setminus\{\mathbf{0}\}$ with $\mathbf{B}\boldsymbol{\xi}=\mathbf{0}$), are equivalent to

$$\boldsymbol{\xi}^\top\mathbf{M}^*\boldsymbol{\xi}=\boldsymbol{\xi}^\top(\mathbf{M}+\mathbf{B}^\top\mathbf{B})\boldsymbol{\xi}=\boldsymbol{\xi}^\top\mathbf{M}\boldsymbol{\xi}+\|\mathbf{B}\boldsymbol{\xi}\|_2^2>0\,,\;(\boldsymbol{\xi}\in\mathbb{R}^k\setminus\{\mathbf{0}\})\,.$$

This condition guarantees that any non-zero velocity being compatible with the hidden constraints (4) results in a positive contribution to the system's kinetic energy [14].

For non-singular $\mathbf{M}^*(q)$, the modified system (9) may be solved w.r.t. $\dot{\mathbf{v}}$ and $\boldsymbol{\lambda}$ resulting in (10) with $\mathbf{M}$, $\mathbf{g}$ being substituted by $\mathbf{M}^*(q)$, $\mathbf{g}^*(q,\mathbf{v},t)$ and the DAE index of (1) is – as before – bounded by three since $\dot{\boldsymbol{\lambda}}=\dot{\boldsymbol{\lambda}}(q,\mathbf{v},t)$ is obtained by differentiation of (10b) w.r.t. t. A more detailed analysis shows, however, that the DAE index of (1) may be less than three if $\mathbf{M}(q)$ is rank deficient (and positive definite at $\ker\mathbf{B}(q)$). As a (pathological) example, we consider equations of motion (1) in a linear space with linear constraints (1c), i.e., $G=\mathbb{R}^k$, $\boldsymbol{\Phi}(\mathbf{q})=\mathbf{B}\mathbf{q}$. If mass matrix $\mathbf{M}$ and force vector $\mathbf{g}$ vanish identically and the constraint matrix is square and non-singular ($m=k$, $\ker\mathbf{B}=\{\mathbf{0}\}$), then (1) is given by

$$\dot{\mathbf{q}}=\mathbf{v}\,,\;\; \mathbf{0}=-\mathbf{B}^\top\boldsymbol{\lambda}\,,\;\; \mathbf{B}\mathbf{q}=\mathbf{0}\,. \tag{11}$$

Differentiating $-\mathbf{B}^\top\boldsymbol{\lambda}=\mathbf{0}$ once and $\mathbf{B}\mathbf{q}=\mathbf{0}$ twice w.r.t. t, we get ordinary differential equations for $\mathbf{q}$, $\mathbf{v}$ and $\boldsymbol{\lambda}$, i.e., the differentiation index of DAE (11) is two [19].

The convergence analysis for generalized-α methods in [1, 3, 9] that is tailored to index-3 DAEs fails in the application to lower index systems like (11). A more refined structural analysis is necessary to separate in the rank deficient case the components of $\boldsymbol{\lambda}$ that are linearly dependent on $\dot{\mathbf{v}}$, see (9), from the ones that are completely defined by $(q,\mathbf{v},t)$:

Assumption 1. Consider equations of motion (1) with a symmetric, positive semi-definite mass matrix $\mathbf{M}(q) \in \mathbb{R}^{k\times k}$ of constant rank $r := \operatorname{rank} \mathbf{M}(q) \leq k$ that is positive definite at the null space of the constraint matrix $\mathbf{B}(q) \in \mathbb{R}^{m\times k}$. We assume that $\mathbf{B}(q)$ has full rank m along the solution and that the 2×2 block matrix at the left hand side of (9) may be transformed to

$$\left(\begin{array}{c|c} \mathbf{M}(q) & \mathbf{B}^\top(q) \\ \hline \mathbf{B}(q) & \mathbf{0} \end{array}\right) = \left(\begin{array}{c|c} \mathbf{U}(q) & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{Q}(q) \end{array}\right) \left(\begin{array}{cc|cc} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}_{k-r} \\ \mathbf{0} & \bar{\mathbf{\Lambda}}(q) & \bar{\mathbf{B}}^\top(q) & \mathbf{0} \\ \hline \mathbf{0} & \bar{\mathbf{B}}(q) & \mathbf{0} & \mathbf{0} \\ \mathbf{I}_{k-r} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right) \left(\begin{array}{c|c} \mathbf{U}^\top(q) & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{Q}^\top(q) \end{array}\right)$$

with non-singular matrices $\mathbf{U}(q) \in \mathbb{R}^{k\times k}$, $\mathbf{Q}(q) \in \mathbb{R}^{m\times m}$ and a 4×4 block matrix with square diagonal blocks of size $k-r$, r, $m-(k-r)$ and $k-r$. The diagonal block $\bar{\mathbf{\Lambda}}(q) \in \mathbb{R}^{r\times r}$ is non-singular since $r = \operatorname{rank} \mathbf{M}(q) = \operatorname{rank} \bar{\mathbf{\Lambda}}(q)$ and the off-diagonal block $\bar{\mathbf{B}}(q) \in \mathbb{R}^{(m-(k-r))\times r}$ has full rank $m-(k-r)$ since $m = \operatorname{rank} \mathbf{B}(q) = \operatorname{rank} \bar{\mathbf{B}}(q) + \operatorname{rank} \mathbf{I}_{k-r}$. The matrix decomposition is assumed to be smooth in the sense that $\mathbf{U}(q)$, $\mathbf{Q}(q)$, $\bar{\mathbf{\Lambda}}(q)$ and $\bar{\mathbf{B}}(q)$ are continuously differentiable w.r.t. $q \in G$.

This structural assumption is motivated by the observation that for constant matrices $\mathbf{M}$, $\mathbf{B}$, the existence of such a transformation is always guaranteed if $\mathbf{B}$ has full rank and $\mathbf{M}$ is symmetric, positive semi-definite and furthermore positive definite at the null space of $\mathbf{B}$:

Lemma 1. *Let matrices $\mathbf{M} \in \mathbb{R}^{k\times k}$ and $\mathbf{B} \in \mathbb{R}^{m\times k}$ be constant with $\operatorname{rank} \mathbf{M} = r \leq k$ and $\operatorname{rank} \mathbf{B} = m$. If $\mathbf{M}$ is symmetric, positive semi-definite and*

$$\mathbf{B}\boldsymbol{\xi} = \mathbf{0} \;\Rightarrow\; \boldsymbol{\xi}^\top \mathbf{M} \boldsymbol{\xi} > 0 \tag{12}$$

for all vectors $\boldsymbol{\xi} \in \mathbb{R}^k \setminus \{\mathbf{0}\}$ then there are non-singular matrices $\mathbf{U} \in \mathbb{R}^{k\times k}$ and $\mathbf{Q} \in \mathbb{R}^{m\times m}$ such that

$$\left(\begin{array}{c|c} \mathbf{M} & \mathbf{B}^\top \\ \hline \mathbf{B} & \mathbf{0} \end{array}\right) = \left(\begin{array}{c|c} \mathbf{U} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{Q} \end{array}\right) \left(\begin{array}{cc|cc} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}_{k-r} \\ \mathbf{0} & \bar{\mathbf{\Lambda}} & \bar{\mathbf{B}}^\top & \mathbf{0} \\ \hline \mathbf{0} & \bar{\mathbf{B}} & \mathbf{0} & \mathbf{0} \\ \mathbf{I}_{k-r} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right) \left(\begin{array}{c|c} \mathbf{U}^\top & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{Q}^\top \end{array}\right) \tag{13}$$

with a non-singular matrix $\bar{\mathbf{\Lambda}} \in \mathbb{R}^{r\times r}$ and a matrix $\bar{\mathbf{B}} \in \mathbb{R}^{(m-(k-r))\times r}$ that has full rank $m-(k-r)$.

Proof. In $\mathbb{R}^k$, there is an orthonormal basis of eigenvectors $\mathbf{u}_i$, $(i = 1, \ldots, k)$, of the symmetric mass matrix $\mathbf{M} \in \mathbb{R}^{k\times k}$ such that the first $k-r$ eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_{k-r}$ span the null space of $\mathbf{M}$, i.e., the eigenspace corresponding to the zero eigenvalues $\mu_1, \ldots, \mu_{k-r}$. Summarizing the eigenvectors in matrices $\bar{\bar{\mathbf{U}}} := \left(\mathbf{u}_1, \ldots, \mathbf{u}_{k-r}\right) \in \mathbb{R}^{k\times(k-r)}$ and $\bar{\mathbf{U}} := \left(\mathbf{u}_{(k-r)+1}, \ldots, \mathbf{u}_k\right) \in \mathbb{R}^{k\times r}$, we get $\mathbf{M}\bar{\bar{\mathbf{U}}} = \mathbf{0}_{k\times(k-r)}$ and $\mathbf{M}\bar{\mathbf{U}} = \bar{\mathbf{U}}\bar{\mathbf{\Lambda}}$ with a non-singular diagonal matrix $\bar{\mathbf{\Lambda}} := \operatorname{diag}\left(\mu_{(k-r)+1}, \ldots, \mu_k\right) \in \mathbb{R}^{r\times r}$ containing the non-vanishing eigenvalues of $\mathbf{M}$.

The column vectors of $\mathbf{B}\bar{\bar{\mathbf{U}}} \in \mathbb{R}^{m\times(k-r)}$ are linearly independent since otherwise there would be a vector $\boldsymbol{\zeta} \in \mathbb{R}^{k-r}$ with $\boldsymbol{\zeta} \neq \mathbf{0}$ and $\mathbf{0} = (\mathbf{B}\bar{\bar{\mathbf{U}}})\boldsymbol{\zeta} = \mathbf{B}(\bar{\bar{\mathbf{U}}}\boldsymbol{\zeta})$. For this vector $\boldsymbol{\zeta}$, we could use assumption (12) with $\boldsymbol{\xi} := \bar{\bar{\mathbf{U}}}\boldsymbol{\zeta} \neq \mathbf{0}$ to get $(\bar{\bar{\mathbf{U}}}\boldsymbol{\zeta})^\top \mathbf{M}(\bar{\bar{\mathbf{U}}}\boldsymbol{\zeta}) > 0$ which contradicts the fact that $(\bar{\bar{\mathbf{U}}}\boldsymbol{\zeta})^\top \mathbf{M}(\bar{\bar{\mathbf{U}}}\boldsymbol{\zeta}) = \boldsymbol{\zeta}^\top(\bar{\bar{\mathbf{U}}}^\top \mathbf{M}\bar{\bar{\mathbf{U}}})\boldsymbol{\zeta}$ and $\ker \mathbf{M} = \operatorname{span} \bar{\bar{\mathbf{U}}}$, i.e., $\mathbf{M}\bar{\bar{\mathbf{U}}} = \mathbf{0}$. Because of $\operatorname{rank} \mathbf{B}\bar{\bar{\mathbf{U}}} = k-r \leq m$, there is a QR factorization

$$\mathbf{B}\bar{\bar{\mathbf{U}}} = \bar{\bar{\mathbf{Q}}} \begin{pmatrix} \bar{\bar{\mathbf{R}}} \\ \mathbf{0} \end{pmatrix}$$

with an orthogonal matrix $\bar{\bar{\mathbf{Q}}} \in \mathbb{R}^{m\times m}$ and a non-singular matrix $\bar{\bar{\mathbf{R}}} \in \mathbb{R}^{(k-r)\times(k-r)}$, see, e.g., [18]. Since

$$\mathbf{Q} := \bar{\bar{\mathbf{Q}}} \begin{pmatrix} \mathbf{0} & \bar{\bar{\mathbf{R}}} \\ \mathbf{I}_{m-(k-r)} & \mathbf{0} \end{pmatrix} \;\Rightarrow\; \mathbf{B}\bar{\bar{\mathbf{U}}} = \mathbf{Q}\begin{pmatrix} \mathbf{0} \\ \mathbf{I}_{k-r} \end{pmatrix},\;\; \mathbf{Q}^{-1}\mathbf{B}\bar{\bar{\mathbf{U}}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{I}_{k-r} \end{pmatrix}, \tag{14}$$

we consider also in matrix $\mathbf{Q}^{-1}\mathbf{B}\bar{\mathbf{U}} \in \mathbb{R}^{m\times r}$ the last $k-r$ rows separately from the remaining ones:

$$\begin{pmatrix} \bar{\mathbf{B}} \\ \bar{\bar{\mathbf{B}}} \end{pmatrix} := \mathbf{Q}^{-1}\mathbf{B}\bar{\mathbf{U}} \;\Rightarrow\; \mathbf{B}\bar{\mathbf{U}} = \mathbf{Q}\begin{pmatrix} \bar{\mathbf{B}} \\ \bar{\bar{\mathbf{B}}} \end{pmatrix} \tag{15}$$

with $\bar{\mathbf{B}} \in \mathbb{R}^{(m-(k-r))\times r}$ and $\bar{\bar{\mathbf{B}}} \in \mathbb{R}^{(k-r)\times r}$. Summarizing (14) and (15), we get an expression for the matrix product $\mathbf{B}\big(\bar{\bar{\mathbf{U}}}, \bar{\mathbf{U}}\big) \in \mathbb{R}^{m\times k}$ that may be used to express the constraint matrix $\mathbf{B} \in \mathbb{R}^{m\times k}$ in terms of the matrices $\mathbf{Q}$, $\bar{\mathbf{B}}$, $\bar{\bar{\mathbf{B}}}$ and the inverse of the orthogonal matrix $\big(\, \bar{\bar{\mathbf{U}}}\ \bar{\mathbf{U}} \,\big) \in \mathbb{R}^{k\times k}$:

$$
\begin{aligned}
\mathbf{B} &= \mathbf{Q}\begin{pmatrix} \mathbf{0} & \bar{\mathbf{B}} \\ \mathbf{I}_{k-r} & \bar{\bar{\mathbf{B}}} \end{pmatrix}\big(\, \bar{\bar{\mathbf{U}}}\ \bar{\mathbf{U}} \,\big)^{-1} = \mathbf{Q}\begin{pmatrix} \mathbf{0} & \bar{\mathbf{B}} \\ \mathbf{I}_{k-r} & \bar{\bar{\mathbf{B}}} \end{pmatrix}\begin{pmatrix} \bar{\bar{\mathbf{U}}}^\top \\ \bar{\mathbf{U}}^\top \end{pmatrix} \\
&= \mathbf{Q}\begin{pmatrix} \mathbf{0} & \bar{\mathbf{B}} \\ \mathbf{I}_{k-r} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \mathbf{I}_{k-r} & \bar{\bar{\mathbf{B}}} \\ \mathbf{0} & \mathbf{I}_r \end{pmatrix}\begin{pmatrix} \bar{\bar{\mathbf{U}}}^\top \\ \bar{\mathbf{U}}^\top \end{pmatrix} = \mathbf{Q}\begin{pmatrix} \mathbf{0} & \bar{\mathbf{B}} \\ \mathbf{I}_{k-r} & \mathbf{0} \end{pmatrix}\mathbf{U}^\top
\end{aligned}
$$

with the non-singular matrix

$$
\mathbf{U} := \big(\, \bar{\bar{\mathbf{U}}}\ \bar{\mathbf{U}} \,\big)\begin{pmatrix} \mathbf{I}_{k-r} & \mathbf{0} \\ \bar{\bar{\mathbf{B}}}^\top & \mathbf{I}_r \end{pmatrix} \in \mathbb{R}^{k\times k}
$$

that transforms the upper left block of the 2×2 matrix at the left hand side of (13) according to

$$
\begin{aligned}
\mathbf{U}\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{\Lambda}} \end{pmatrix}\mathbf{U}^\top &= \big(\, \bar{\bar{\mathbf{U}}}\ \bar{\mathbf{U}} \,\big)\begin{pmatrix} \mathbf{I}_{k-r} & \mathbf{0} \\ \bar{\bar{\mathbf{B}}}^\top & \mathbf{I}_r \end{pmatrix}\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{\Lambda}} \end{pmatrix}\begin{pmatrix} \mathbf{I}_{k-r} & \bar{\bar{\mathbf{B}}} \\ \mathbf{0} & \mathbf{I}_r \end{pmatrix}\begin{pmatrix} \bar{\bar{\mathbf{U}}}^\top \\ \bar{\mathbf{U}}^\top \end{pmatrix} \\
&= \big(\, \bar{\bar{\mathbf{U}}}\ \bar{\mathbf{U}} \,\big)\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{\Lambda}} \end{pmatrix}\begin{pmatrix} \bar{\bar{\mathbf{U}}}^\top \\ \bar{\mathbf{U}}^\top \end{pmatrix} = \big(\, \mathbf{0}\ \ \bar{\mathbf{U}}\bar{\mathbf{\Lambda}} \,\big)\begin{pmatrix} \bar{\bar{\mathbf{U}}}^\top \\ \bar{\mathbf{U}}^\top \end{pmatrix} = \mathbf{M}\,\big(\, \bar{\bar{\mathbf{U}}}\ \bar{\mathbf{U}} \,\big)\begin{pmatrix} \bar{\bar{\mathbf{U}}}^\top \\ \bar{\mathbf{U}}^\top \end{pmatrix} = \mathbf{M}\,.
\end{aligned}
$$

To complete the proof, we observe that the third block row of the non-singular 4×4 block matrix in (13) contains only one non-zero block. Therefore, this block has to have full rank: $\operatorname{rank}\bar{\mathbf{B}} = m-(k-r)$. □

The block structure of the decomposition according to Assumption 1 allows to decouple the dynamical equations (1b) by left multiplication with matrix $\mathbf{U}^{-1}(q)$. Splitting the vectors $\dot{\mathbf{v}}$, $\mathbf{g}$ and $\boldsymbol{\lambda}$ in (1b) such that

$$
\mathbf{U}^\top(q)\,\dot{\mathbf{v}} = \begin{pmatrix} \dot{\bar{\bar{\mathbf{v}}}} \\ \dot{\bar{\mathbf{v}}} \end{pmatrix},\ \ \mathbf{U}^{-1}(q)\,\mathbf{g} = \begin{pmatrix} \bar{\bar{\mathbf{g}}} \\ \bar{\mathbf{g}} \end{pmatrix},\ \ \mathbf{Q}^\top(q)\,\boldsymbol{\lambda} = \begin{pmatrix} \bar{\boldsymbol{\lambda}} \\ \bar{\bar{\boldsymbol{\lambda}}} \end{pmatrix}, \tag{16}
$$

the decoupled equations may be written as

$$
\mathbf{0} = -\bar{\bar{\mathbf{g}}}(q,\mathbf{v},t) - \bar{\bar{\boldsymbol{\lambda}}}\,, \tag{17a}
$$

$$
\bar{\mathbf{\Lambda}}(q)\dot{\bar{\mathbf{v}}} = -\bar{\mathbf{g}}(q,\mathbf{v},t) - \bar{\mathbf{B}}^\top(q)\bar{\boldsymbol{\lambda}}\,. \tag{17b}
$$

In (17), the algebraic components $\bar{\bar{\boldsymbol{\lambda}}} \in \mathbb{R}^{k-r}$ are explicitly defined as a function of the differential solution components q and $\mathbf{v}$. This structure is typical of index-1 DAEs and allows to bound the global error in $\bar{\bar{\boldsymbol{\lambda}}}$ directly in terms of the global errors in components q and $\mathbf{v}$. Using the notation of [3, 9], we define these global errors $\mathbf{e}_n^{(\bullet)}$ for all solution components from linear spaces by $(\bullet)(t_n) = (\bullet)_n + \mathbf{e}_n^{(\bullet)}$ and use $q(t_n) = q_n \circ \exp(\widetilde{\mathbf{e}}_n^q)$ to define the global error in components $q \in G$. Then we get from (17a) and from the corresponding equation for the numerical solution at $t = t_{n+1}$, see (3e), the error estimate

$$
\|\mathbf{e}_{n+1}^{\bar{\bar{\boldsymbol{\lambda}}}}\| = \mathcal{O}(1)(\|\mathbf{e}_{n+1}^q\| + \|\mathbf{e}_{n+1}^{\mathbf{v}}\|)\,. \tag{18}
$$

The global errors in the algebraic solution components $\dot{\bar{\mathbf{v}}} \in \mathbb{R}^r$ and $\bar{\boldsymbol{\lambda}} \in \mathbb{R}^{m-(k-r)}$ may be studied following the convergence analysis in [1, 3, 9] since the coefficient $\bar{\mathbf{\Lambda}} \in \mathbb{R}^{r\times r}$ of $\dot{\bar{\mathbf{v}}}$ is symmetric and positive definite and the reduced constraint matrix $\bar{\mathbf{B}} \in \mathbb{R}^{(m-(k-r))\times r}$ has full rank $m-(k-r)$. Using notations

$$
\bar{\mathbf{P}}(q) := \mathbf{I} - [\bar{\mathbf{\Lambda}}^{-1}\bar{\mathbf{B}}^\top\bar{\mathbf{S}}^{-1}\bar{\mathbf{B}}](q) \ \text{ with } \ \bar{\mathbf{S}}(q) := [\bar{\mathbf{B}}\bar{\mathbf{\Lambda}}^{-1}\bar{\mathbf{B}}^\top](q)
$$

and $\mathbf{e}_n^{(\mathbf{C}\,\bullet)} := \mathbf{C}(q(t_n))\mathbf{e}_n^{(\bullet)}$ for any matrix valued function $\mathbf{C} = \mathbf{C}(q)$, see [3], we get error estimates

$$
\mathbf{e}_{n+1}^{\bar{\mathbf{P}}\dot{\bar{\mathbf{v}}}} = \mathcal{O}(1)(\|\mathbf{e}_{n+1}^q\| + \|\mathbf{e}_{n+1}^{\mathbf{v}}\| + h\|\mathbf{e}_{n+1}^{\bar{\boldsymbol{\lambda}}}\|)\,, \tag{19a}
$$

$$
\mathbf{e}_{n+1}^{\bar{\mathbf{B}}\dot{\bar{\mathbf{v}}}} + \mathbf{e}_{n+1}^{\bar{\mathbf{S}}\bar{\boldsymbol{\lambda}}} = \mathcal{O}(1)(\|\mathbf{e}_{n+1}^q\| + \|\mathbf{e}_{n+1}^{\mathbf{v}}\| + h\|\mathbf{e}_{n+1}^{\bar{\boldsymbol{\lambda}}}\|) \tag{19b}
$$

from (17b) and from the corresponding equation for the numerical solution at $t = t_{n+1}$, see (3e). Note, that the left hand side of (19a) does not contain a term $\mathbf{e}_{n+1}^{\bar{\boldsymbol{\lambda}}}$ since $\bar{\mathbf{P}}(q)\bar{\boldsymbol{\Lambda}}^{-1}(q)\bar{\mathbf{B}}^{\top}(q) \equiv \mathbf{0}$.

Finally, the algebraic solution components $\bar{\bar{\dot{\mathbf{v}}}} \in \mathbb{R}^{k-r}$ do not appear at all in the decoupled equations (17). Therefore, the global error analysis for these components can not be based on the dynamical equations (1b) and their time discrete counterpart (3e).

As in [3, 9], we define the global error $\mathbf{e}_n^{\mathbf{a}}$ by $\dot{\mathbf{v}}(t_n + \Delta_\alpha h) = \mathbf{a}_n + \mathbf{e}_n^{\mathbf{a}}$ with $\Delta_\alpha = \alpha_m - \alpha_f$ to get in (3d) a local truncation error of size $\mathcal{O}(h^2)$. The splitting of $\mathbf{U}^{\top}(q)\dot{\mathbf{v}}$ in components $\bar{\bar{\dot{\mathbf{v}}}}$, $\bar{\dot{\mathbf{v}}}$, see (16), and the linear relation between components $\mathbf{a}$ and $\dot{\mathbf{v}}$ suggests to split $\mathbf{U}^{\top}\big(q(t_n)\big)\mathbf{e}_n^{\mathbf{a}} \in \mathbb{R}^k$ as well into components $\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}} \in \mathbb{R}^{k-r}$ and $\mathbf{e}_n^{\bar{\mathbf{a}}} \in \mathbb{R}^r$ to get

$$
\begin{aligned}
(1-\alpha_m)\mathbf{e}_{n+1}^{\bar{\mathbf{P}}\bar{\mathbf{a}}} + \alpha_m \mathbf{e}_n^{\bar{\mathbf{P}}\bar{\mathbf{a}}} &= \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)\,, && \text{(20a)}\\
(1-\alpha_m)\mathbf{e}_{n+1}^{\bar{\mathbf{B}}\bar{\mathbf{a}}} + \alpha_m \mathbf{e}_n^{\bar{\mathbf{B}}\bar{\mathbf{a}}} + (1-\alpha_f)\mathbf{e}_{n+1}^{\bar{\mathbf{S}}\bar{\boldsymbol{\lambda}}} + \alpha_f \mathbf{e}_n^{\bar{\mathbf{S}}\bar{\boldsymbol{\lambda}}} &= \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)\,, && \text{(20b)}
\end{aligned}
$$

see (3d) and (19) and [3, Lemma 5]. The terms ε_n, ε_{n+1} in the right hand side of (20) summarize higher order error terms, $\varepsilon_n := \|\mathbf{e}_n^q\| + \|\mathbf{e}_n^{\mathbf{v}}\| + h\|\mathbf{e}_n^{\mathbf{a}}\| + h\|\mathbf{e}_n^{\boldsymbol{\lambda}}\|$.

To estimate error components in normal direction to the constraint manifold $\mathfrak{M} = \{\, q \in G \,:\, \boldsymbol{\Phi}(q) = \mathbf{0}\,\}$, we studied in [3] time discrete approximations of the hidden constraints (5) to prove

$$
\mathbf{0} = \mathbf{B}\big(q(t_n)\big)\boldsymbol{\Delta}_h \mathbf{e}_n^q + \mathbf{Z}\big(q(t_n)\big)\big(\mathbf{e}_n^q, \mathbf{v}(t_n)\big) + \mathcal{O}(h)(\|\mathbf{e}_n^q\| + \|\boldsymbol{\Delta}_h \mathbf{e}_n^q\|) \tag{21}
$$

with $\boldsymbol{\Delta}_h \mathbf{e}_n^q := (\mathbf{e}_{n+1}^q - \mathbf{e}_n^q)/h$. For rank deficient mass matrices, the vector

$$
\mathbf{r}_{\mathbf{n}}^{\mathbf{B}} := \frac{1}{h}\Big(\mathbf{B}\big(q(t_n)\big)\big(\boldsymbol{\Delta}_h \mathbf{e}_n^q - h(0.5-\beta)\mathbf{e}_n^{\mathbf{a}} - h\beta\mathbf{e}_{n+1}^{\mathbf{a}}\big) + \mathbf{Z}\big(q(t_n)\big)\big(\mathbf{e}_n^q, \mathbf{v}(t_n)\big)\Big) \in \mathbb{R}^m \tag{22}
$$

that was defined in [3, Section 3.5] is split into components $\bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}} \in \mathbb{R}^{m-(k-r)}$ and $\bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}} \in \mathbb{R}^{k-r}$ according to

$$
\begin{pmatrix} \bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}} \\ \bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}} \end{pmatrix} := \mathbf{Q}^{-1}(q(t_n))\,\mathbf{r}_{\mathbf{n}}^{\mathbf{B}}\,. \tag{23}
$$

Taking into account the 2×2 block structure of matrix $\mathbf{Q}^{-1}\mathbf{B}(\mathbf{U}^{\top})^{-1} \in \mathbb{R}^{m \times k}$ in Assumption 1, we get

$$
[\mathbf{Q}^{-1}\mathbf{B}]\big(q(t_n)\big)\mathbf{e}_n^{\mathbf{a}} = [\mathbf{Q}^{-1}\mathbf{B}(\mathbf{U}^{\top})^{-1}]\big(q(t_n)\big)\,\mathbf{U}^{\top}\big(q(t_n)\big)\mathbf{e}_n^{\mathbf{a}} = \begin{pmatrix} \mathbf{0} & \bar{\mathbf{B}}\big(q(t_n)\big) \\ \mathbf{I}_{k-r} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{e}_n^{\bar{\bar{\mathbf{a}}}} \\ \mathbf{e}_n^{\bar{\mathbf{a}}} \end{pmatrix}. \tag{24}
$$

Therefore, error component $\bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}}$ is decoupled from $\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}}$, $\mathbf{e}_{n+1}^{\bar{\bar{\mathbf{a}}}}$ in the sense that

$$
\bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}} + (0.5-\beta)\mathbf{e}_n^{\bar{\mathbf{B}}\bar{\mathbf{a}}} + \beta\mathbf{e}_{n+1}^{\bar{\mathbf{B}}\bar{\mathbf{a}}} = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)\,, \tag{25a}
$$

see (21), (22)–(24) and [3, Lemma 6]. The corresponding estimate for error component $\bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}}$ is given by

$$
\bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}} + (0.5-\beta)\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}} + \beta\mathbf{e}_{n+1}^{\bar{\bar{\mathbf{a}}}} = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)\,. \tag{25b}
$$

To complete the error analysis for the algebraic solution components, we follow step-by-step the analysis in the proof of [3, Lemma 6] to get error estimates for the differences $\bar{\mathbf{r}}_{\mathbf{n+1}}^{\mathbf{B}} - \bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}}$ and $\bar{\bar{\mathbf{r}}}_{\mathbf{n+1}}^{\mathbf{B}} - \bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}}$. Taking into account again the splitting (23) of $\mathbf{r}_{\mathbf{n}}^{\mathbf{B}}$ into components $\bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}}$, $\bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}}$ and the 2×2 block structure of matrix $\mathbf{Q}^{-1}\mathbf{B}(\mathbf{U}^{\top})^{-1}$, see (24), we obtain

$$
\begin{aligned}
\bar{\mathbf{r}}_{\mathbf{n+1}}^{\mathbf{B}} - \bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}} &= (1-\gamma)\mathbf{e}_n^{\bar{\mathbf{B}}\bar{\mathbf{a}}} + \gamma\mathbf{e}_{n+1}^{\bar{\mathbf{B}}\bar{\mathbf{a}}} + \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)\,, && \text{(26a)}\\
\bar{\bar{\mathbf{r}}}_{\mathbf{n+1}}^{\mathbf{B}} - \bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}} &= (1-\gamma)\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}} + \gamma\mathbf{e}_{n+1}^{\bar{\bar{\mathbf{a}}}} + \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)\,. && \text{(26b)}
\end{aligned}
$$

With the matrix decomposition according to Assumption 1, the leading error terms in the algebraic solution components $\dot{\mathbf{v}}$, $\mathbf{a}$ and $\boldsymbol{\lambda}$ may be studied separately for an r-dimensional subsystem of full rank (error terms $\mathbf{e}_n^{\bar{\mathbf{P}}\bar{\dot{\mathbf{v}}}}$, $\mathbf{e}_n^{\bar{\mathbf{B}}\bar{\dot{\mathbf{v}}}}$, $\mathbf{e}_n^{\bar{\mathbf{P}}\bar{\mathbf{a}}}$, $\mathbf{e}_n^{\bar{\mathbf{B}}\bar{\mathbf{a}}}$, $\bar{\mathbf{r}}_{\mathbf{n}}^{\mathbf{B}}$, $\mathbf{e}_n^{\bar{\mathbf{S}}\bar{\boldsymbol{\lambda}}}$) and for the $(k-r)$-dimensional null space of $\mathbf{M}(q)$ (error terms $\mathbf{e}_n^{\bar{\bar{\dot{\mathbf{v}}}}}$, $\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}}$, $\bar{\bar{\mathbf{r}}}_{\mathbf{n}}^{\mathbf{B}}$,

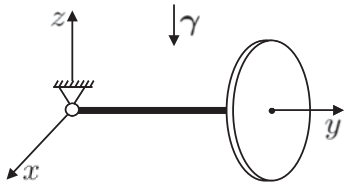

Figure 3: Heavy top benchmark [8, 17].

$\mathbf{e}_n^{\bar{\bar{\boldsymbol{\lambda}}}}$). In (20), (25) and (26), the error estimates for both subsystems are coupled by higher order error terms ε_n, ε_{n+1}. Note, that the two identity matrices $\mathbf{I}_{k-r}$ in Assumption 1 correspond to error terms $\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}}$ and $\mathbf{e}_n^{\bar{\bar{\boldsymbol{\lambda}}}}$ without any coefficients like the matrices $\bar{\mathbf{P}}$, $\bar{\mathbf{B}}$ and $\bar{\mathbf{S}}$ in $\mathbf{e}_n^{\bar{\mathbf{P}}\bar{\mathbf{a}}}$, $\mathbf{e}_n^{\bar{\mathbf{B}}\bar{\mathbf{a}}}$ and $\mathbf{e}_n^{\bar{\mathbf{S}}\bar{\boldsymbol{\lambda}}}$.

The four error estimates (20a), (20b), (25a) and (26a) for the r-dimensional subsystem of full rank correspond one-by-one to the error estimates for the algebraic solution components that were derived in [3] for equations of motion (1) with full-rank mass matrix $\mathbf{M}(q)$. The essential new results for systems with rank-deficient mass matrix are given in (18), (25b) and (26b). Summarizing (25b) and (26b) in

$$\|(\bar{\bar{\mathbf{T}}}_+ \otimes \mathbf{I}_{k-r}) \begin{pmatrix} \bar{\bar{\mathbf{r}}}^{\mathbf{B}}_{\mathbf{n+1}} \\ \mathbf{e}^{\bar{\bar{\mathbf{a}}}}_{n+1} \end{pmatrix} - (\bar{\bar{\mathbf{T}}}_0 \otimes \mathbf{I}_{k-r}) \begin{pmatrix} \bar{\bar{\mathbf{r}}}^{\mathbf{B}}_{\mathbf{n}} \\ \mathbf{e}^{\bar{\bar{\mathbf{a}}}}_{n} \end{pmatrix} \| = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2) \tag{27}$$

with

$$\bar{\bar{\mathbf{T}}}_+ = \begin{pmatrix} 0 & -\beta \\ 1 & -\gamma \end{pmatrix}, \quad \bar{\bar{\mathbf{T}}}_0 = \begin{pmatrix} 1 & 0.5-\beta \\ 1 & 1-\gamma \end{pmatrix},$$

the analysis of the coupled error propagation in components $\mathbf{e}_n^q$, $\mathbf{e}_n^{\mathbf{v}}$, $\mathbf{e}_n^{\bar{\mathbf{P}}\bar{\mathbf{a}}}$, $\mathbf{e}_n^{\bar{\mathbf{B}}\bar{\mathbf{a}}}$, $\mathbf{e}_n^{\bar{\bar{\mathbf{a}}}}$, $\bar{\mathbf{r}}^{\mathbf{B}}_{\mathbf{n}}$, $\bar{\bar{\mathbf{r}}}^{\mathbf{B}}_{\mathbf{n}}$, $\mathbf{e}_n^{\bar{\mathbf{S}}\bar{\boldsymbol{\lambda}}}$ and $\mathbf{e}_n^{\bar{\bar{\boldsymbol{\lambda}}}}$ yields exactly the same convergence result as in the full rank case, see [3, Theorem 1] since the contractivity condition $\varrho(\bar{\bar{\mathbf{T}}}_+^{-1}\bar{\bar{\mathbf{T}}}_0) < 1$ is satisfied whenever $\gamma > 1/2$ and $\beta > \gamma/2$, see [1, Lemma 1] and [3, Lemma 8].

5 CONCLUSIONS

The recently developed one-step error recursion for generalized-α time integration methods is a powerful tool to analyse in the constrained case the asymptotic behaviour for small time step sizes. In numerical tests, we observed that the projection of the velocity vector onto the manifold that is defined by the hidden constraints at the level of velocity coordinates may cause transient oscillations of large amplitude in the Lagrange multipliers. The one-step error recursion shows that this undesired numerical behaviour is caused by order reduction resulting from the velocity projection. Furthermore, we generalized the one-step error recursion by a detailed structural analysis to constrained systems with a rank deficient mass matrix that is symmetric and positive definite at the null space of the constraint matrix.

APPENDIX: HEAVY TOP BENCHMARK PROBLEM

A top that rotates in a gravity field is a classical test problem for studying and comparing different parameterizations of finite rotations in rigid body dynamics. As in [17], we consider a top rotating about a fixed point, see Fig. 3. In this appendix, we follow the presentation of the heavy top benchmark problem in [3, Section 5] using model parameters from [9, Section 7.1].

In the inertial frame, the position and orientation of the top are represented by the position $\mathbf{x} \in \mathbb{R}^3$ of the center of mass and by the rotation matrix $\mathbf{R} \in \mathrm{SO}(3)$. The set $\mathbb{R}^3 \times \mathrm{SO}(3)$ with the composition operation

$$\big(\mathbf{x}_1, \mathbf{R}_1\big) \circ \big(\mathbf{x}_2, \mathbf{R}_2\big) = \big(\mathbf{x}_1 + \mathbf{x}_2, \mathbf{R}_1\mathbf{R}_2\big)$$

defines a 6-dimensional Lie group $G \subset \mathbb{R}^{12}$ with elements $q = (\mathbf{x}, \mathbf{R})$. The kinematic relations (1a) are given by

$$\dot{\mathbf{x}} = \mathbf{u}, \quad \dot{\mathbf{R}} = \mathbf{R}\widetilde{\boldsymbol{\Omega}} \tag{28a}$$

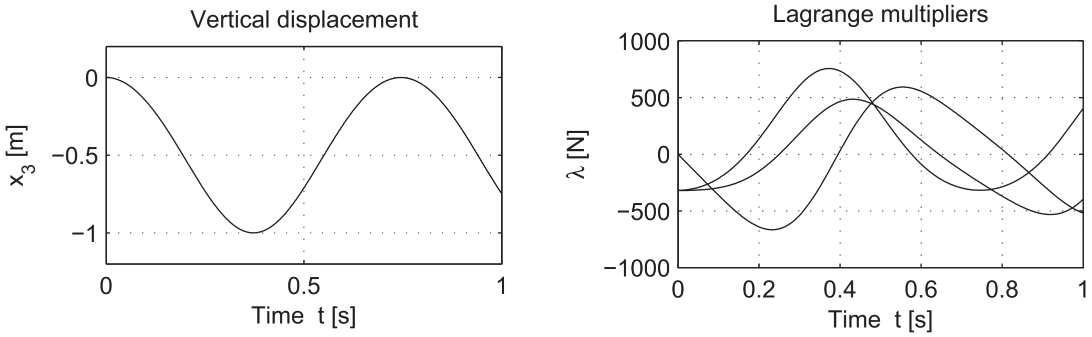

Figure 4: Heavy top benchmark: Reference solution, computed with $h = 2.5 \times 10^{-5}$ s, see [3].

with $\mathbf{u} \in \mathbb{R}^3$ denoting the translational velocity in the inertial frame and a skew symmetric matrix

$$\widetilde{\mathbf{\Omega}} := \begin{pmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & \Omega_1 & 0 \end{pmatrix} \in \mathbb{R}^{3\times 3}$$

that represents the angular velocity $\mathbf{\Omega} = (\,\Omega_1,\, \Omega_2,\, \Omega_3\,)^\top \in \mathbb{R}^3$. Vectors $\mathbf{u}$ and $\mathbf{\Omega}$ are summarized in the velocity vector $\mathbf{v} := (\,\mathbf{u}^\top,\, \mathbf{\Omega}^\top\,)^\top \in \mathbb{R}^6$. In this absolute coordinate formulation, the equations of motion are given by

$$\begin{aligned} m\ddot{\mathbf{x}} - \boldsymbol{\lambda} &= m\boldsymbol{\gamma}\,, && (28\text{b}) \\ \mathbf{J}\dot{\mathbf{\Omega}} + \mathbf{\Omega} \times \mathbf{J}\mathbf{\Omega} + \widetilde{\mathbf{X}}\mathbf{R}^\top \boldsymbol{\lambda} &= \mathbf{0}\,, && (28\text{c}) \\ -\mathbf{x} + \mathbf{R}\mathbf{X} &= \mathbf{0}\,. && (28\text{d}) \end{aligned}$$

with m denoting the mass of the top and the inertia tensor $\mathbf{J}$ that is defined with respect to the center of mass. The gravity forces are given by $\boldsymbol{\gamma} \in \mathbb{R}^3$.

To fix the tip of the top at the origin, we introduce the position $\mathbf{X}$ of the center of mass in the body-fixed frame and get the $m = 3$ holonomic constraints (28d). The corresponding Lagrange multipliers are given by $\boldsymbol{\lambda} \in \mathbb{R}^3$. Due to these constraints, the motion is restricted to a 3-dimensional submanifold of G and we have

$$\mathbf{M} = \begin{pmatrix} m\mathbf{I}_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{J} \end{pmatrix}, \quad \mathbf{g} = \begin{pmatrix} -m\boldsymbol{\gamma} \\ \mathbf{\Omega} \times \mathbf{J}\mathbf{\Omega} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} -\mathbf{I}_3 & -\mathbf{R}\widetilde{\mathbf{X}} \end{pmatrix}.$$

Omitting all physical units, the model data are given by $\mathbf{X} = (\,0\,,\,1\,,\,0\,)^\top$, $\boldsymbol{\gamma} = (\,0\,,\,0\,,\,-9.81\,)^\top$, $m = 15.0$ and $\mathbf{J} = \mathrm{diag}\,(\,0.234375\,,\,0.46875\,,\,0.234375\,)$. The (consistent) initial values are set to $\mathbf{x}(0) = \mathbf{X}$, $\mathbf{R}(0) = \mathbf{I}_3$, $\mathbf{u}(0) = -\widetilde{\mathbf{X}}\mathbf{\Omega}(0)$ and $\mathbf{\Omega}(0) = (\,0\,,\,150\,,\,-4.61538\,)^\top$. Fig. 4 shows component $x_3(t)$ and the Lagrange multipliers $\boldsymbol{\lambda}(t)$ of the reference solution that is computed by the stabilized index-2 formulation [3] using the small time step size $h = 2.5 \times 10^{-5}$ s.

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