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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.

Keywords: Generalized-α method; Lie group time integration; Velocity projection

1. Introduction

Backward differentiation formulae (BDF) and Newmark type methods are the most popular classes of time integration methods in industrial multibody system simulation [1, 2]. 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 [3]. 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 [4] 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 [2, 5, 6], see also Ref. [7]. Index reduction techniques [3, 8, 9] that are a quasi-standard for BDF solvers in industrial multibody system simulation [1] have been proposed as well for Newmark type methods [10, 11], see also Ref. [12], but implementations without index reduction still dominate in industrial simulation tools [2, 6].

An extension of generalized-α methods to mechanical systems that have a configuration space with Lie group structure has been proposed in Ref. [13]. 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 [3, 14]. 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.

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time t, see Refs. [3, 8].

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 [15], we have studied the error propagation in generalized-α methods for index-3 DAEs on Lie groups in great detail [12, 16, 17]. 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 [12].

In the present paper, we recall basic aspects of the generalized-α Lie group method (Sec. 2) and use recently obtained convergence results to study the influence of velocity projections on the accuracy of the numerical solution (Sec. 3). In contrast to known error estimates for projection techniques in DAE time integration [14, 18], 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.

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

$$\dot{q} = DL_q(e)\cdot \mathbf{v}, \tag{1a}$$

$$\mathbf{M}(q)\dot{\mathbf{v}} = -\mathbf{g}(q,\mathbf{v},t) - \mathbf{B}^{\top}(q)\boldsymbol{\lambda}, \tag{1b}$$

$$\boldsymbol{\Phi}(q) = 0 \tag{1c}$$

with the velocity vector $\mathbf{v} \in \mathbb{R}^k$ and an invertible linear mapping $(\tilde{\cdot}) : \mathbb{R}^k \to T_eG, \mathbf{v} \mapsto \tilde{\mathbf{v}}$ Here, $e \in G$ is the identity element and $T_q G$ denotes the tangent space of G at point $q \in G$, see Refs. [13, 17] 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 $T_q G$ 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 Eq. (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

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

with $D\boldsymbol{\Phi}(q)\cdot(DL_q(e)\cdot\tilde{\boldsymbol{w}})$ denoting the directional derivative of $\boldsymbol{\Phi}: G \mapsto \mathbb{R}^m$ evaluated at $q \in G$ in the direction $DL_q(e)\cdot\tilde{\boldsymbol{w}} \in T_q G$. 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. For simplicity, we restrict ourselves to scleronomic constraints Eq. (1c) throughout the present paper. All results remain, however, valid as well in the case of rheonomic constraints $\boldsymbol{\Phi}(q,t) = 0$ 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 Eq. (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 Eqs. (1). In linear spaces, the discretization of the kinematic Eq. (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

$$q(t+h) = q(t)\circ\exp\left(h\tilde{\mathbf{v}}(\mathrm{t}) + \frac{h^2}{2}\tilde{\dot{\mathbf{v}}}(t) + \mathcal{O}(h^3)\right),$$

$(h \to 0)$, with the exponential map $\exp : \mathfrak{g} \to G$. For matrix Lie groups G, this exponential map is formally given by its series expansion $\exp(\tilde{\mathbf{w}}) = \sum_i \tilde{\mathbf{w}}^i / i!$. As proposed in Ref. [13], 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

$$q_{n+1} = q_n \circ \exp(h\Delta\mathbf{q}_n), \tag{3a}$$

$$\Delta\mathbf{q}_n = \mathbf{v}_n + (0.5-\beta)h\mathbf{a}_n + \beta h\mathbf{a}_{n+1}, \tag{3b}$$

$$\mathbf{v}_{n+1} = \mathbf{v}_n + (1-\gamma)h\mathbf{a}_n + \gamma h\mathbf{a}_{n+1}, \tag{3c}$$

$$(1-\alpha_m)\mathbf{a}_{n+1} + \alpha_m\mathbf{a}_n = (1-\alpha_f)\dot{\mathbf{v}}_{n+1} + \alpha_f\dot{\mathbf{v}}_n \tag{3d}$$

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

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

$$\boldsymbol{\Phi}(q_{n+1}) = 0. \tag{3f}$$

In linear spaces, the update Eq. (3a) for the position coordinates is simplified to $\mathbf{q}_{n+1} = \mathbf{q}_n + h\,\Delta\mathbf{q}_n$. Method Eqs. (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 [4]. 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 Eqs. (1) in linear spaces were studied in great detail, see, e.g., Ref. [14] for a compact summary. Generalizing these classical results to the Lie group setting in Eqs. (1), we get *hidden* constraints at the level of velocity coordinates differentiating Eq. (1c) w.r.t. t:

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Phi}\big(q(t)\big) = D\boldsymbol{\Phi}\big(q(t)\big)\cdot\dot{q}(t) \\ &= D\boldsymbol{\Phi}(q)\cdot\big(DL_q(e)\cdot\tilde{\mathbf{v}}\big) = \mathbf{B}(q)\mathbf{v} \end{aligned} \tag{4}$$

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

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

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

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

see Ref. [12]. 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 Eqs. (3) discretizes the equations of motion Eqs. (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 Eqs. (4) and (5). If the original constraints Eq. (1c) are simply substituted by Eq. (4) or by Eq. (5), we get the index-2 formulation or the index-1 formulation of the equations of motion [14]. In contrast to the numerical solution q_{n+1} in the generalized-α method Eqs. (3) that remains for all time steps $t_n \to t_{n+1} = t_n + h$ in the constraint manifold $\mathfrak{M} := \{q \in G : \boldsymbol{\Phi}(q) = 0\}$, see Eq. (3f), there is no guarantee that the holonomic constraints Eq. (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.

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 Refs. [14, 18]. 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 $\min\{\|\boldsymbol{dq}\| : \boldsymbol{\Phi}(\mathbf{q}_{n+1} + \mathbf{dq}) = 0\}$ may be generalized to

$$q_n \to q_{n+1} \circ \exp\big(\widetilde{\mathbf{dq}}_{n+1}\big) \tag{6a}$$

with

$$\mathbf{dq}_{n+1} := \operatorname{argmin}\Big\{\|\,\mathbf{dq}\,\| : \boldsymbol{\Phi}\Big(q_{n+1} \circ \exp\big(\widetilde{\mathbf{dq}}\big)\Big) = 0\Big\} \tag{6b}$$

see also the work of Terze et al. [19] 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 Eqs. (6), by

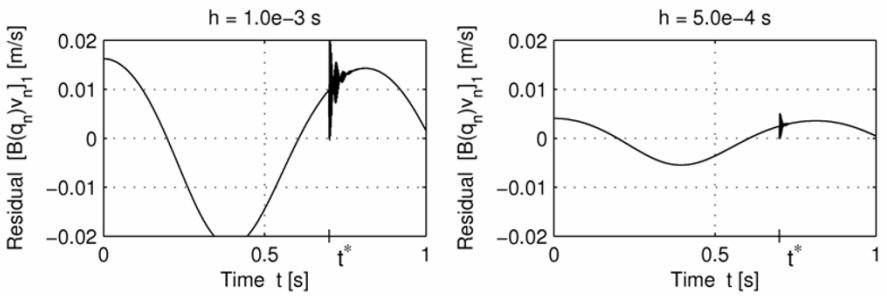
$$\mathbf{v}_{n+1} \to \mathbf{v}_{n+1} + \mathbf{dv}_{n+1} \tag{7a}$$

with

$$\mathbf{dv}_{n+1} := \operatorname{argmin}\big\{\|\,\mathbf{dv}\,\| : \mathbf{B}(q)\big(\mathbf{v}_{n+1} + \mathbf{dv}\big) = 0\big\}. \tag{7b}$$

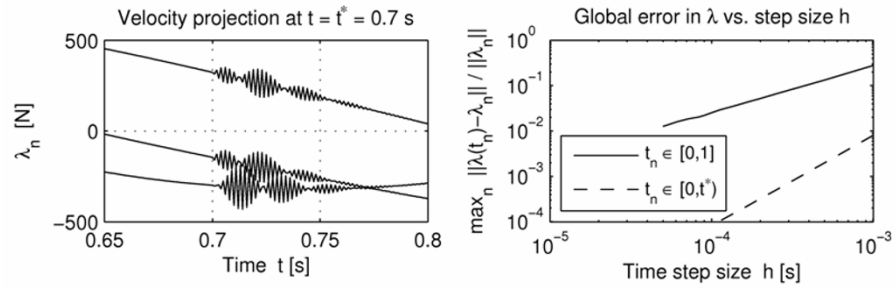
The combination of index reduction and projection techniques is well established in DAE time integration of higher index systems [14]. The extra errors being introduced by the projection of $q_{n+1}, \mathbf{v}_{n+1}$, to $\mathfrak{M}$ and $T_q\mathfrak{M}$ according to Eqs. (6) and (7) remain in the 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 $\mathbf{v}(t) \in T_{q(t)}\mathfrak{M}, (t \ge t_0)$, 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 Eqs. (6) and (7) remain in the size of the local error $\mathcal{O}(h^{p+1})$, see Ref. [14, Sec. VII.2].

The drift-off effect is typical of index reduced formulations and does not affect the generalized-α method Eqs. (3) that discretizes the original Lie group index-3 DAE directly resulting in $\boldsymbol{\Phi}(q_{n+1}) = 0$, see Eq. (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 Eqs. (3) with algorithmic parameters according to Ref. [4] and a damping ratio at infinity of $\rho_\infty = 0.9$ to the heavy top benchmark problem [2, 13, 17]. The equations of motion and all model parameters are given in the appendix below. The equations are formulated in



(a) (b)

Fig. 1. Heavy top benchmark [2, 17], generalized-α method (3) with $h = 1.0 \times 10^{-3}$ s (a) and; $h = 5.0 \times 10^{-4}$ s (b) first component of the residual in hidden constraints (4). Velocity projection at $t = t^* = 0.7$ s .



(a) (b)

Fig. 2. Heavy top benchmark [2, 17], generalized-α method (3), velocity projection at $t = t^* = 0.7$ s . (a) Numerical solution $\boldsymbol{\lambda}_n$ for $h = 1.0 \times 10^{-3}$ s , $t \in [0.65\text{s}, 0.8\text{s}]$; (b) maximum of the norm of global errors in $\boldsymbol{\lambda}$ in a time interval that contains t^* (Solid line) and in the subinterval $[0, t^*]$ (Dashed line).

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 (Fig. 1(a)) and $h = h_0 / 2$ (Fig. 1(b)). 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 Eq. (4), the generalized-α method Eqs. (3) with reasonable starting values [12] 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 Eq. (4) by a projection of $\mathbf{v}_{n+1}$ to the tangential space $T_{q_{n+1}}\mathfrak{M}$ according to Eqs. (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

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

onto the tangential space $T_q\mathfrak{M}$ at $q = q_{n+1}$, see also Refs. [14, 20] 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 Eqs. (3).

The test results in Fig. 1 and in the left plot of Fig. 2 show, however, oscillating constraint residuals of large amplitude for a velocity projection at $t_n = t^* = 0.7$ s that 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

$$\mathbf{E}_{n+1} = \left(\left(\mathbf{T}_+^{-1}\mathbf{T}_0 \right) \otimes \mathbf{I}_m \right) \mathbf{E}_n \tag{8}$$

with

$$\mathbf{E}_n := \begin{pmatrix} \frac{1}{h}\mathbf{B}(q_n)\mathbf{v}_n + h\mathbf{B}\big(q(t_n)\big)\mathbf{r}(t_n) + \zeta_n \\ \Big[\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^{\top}\Big]\big(q(t_n)\big)\big(\boldsymbol{\lambda}(t_n) - \boldsymbol{\lambda}_n\big) \\ \mathbf{B}\big(q(t_n)\big)\big(\dot{\mathbf{v}}(t_n + \Delta_\alpha h) - \mathbf{a}_n\big) \end{pmatrix},$$

$$\tilde{\boldsymbol{r}}(t) = \big(2(1 - 6\beta - 3\Delta_\alpha)\tilde{\ddot{\mathbf{v}}}(t) + \tilde{\mathbf{v}}(t)\tilde{\ddot{\mathbf{v}}}(t) - \tilde{\ddot{\mathbf{v}}}(t)\tilde{\mathbf{v}}(t)\big)/12$$

and a vector $\zeta_n = \mathcal{O}(h^2)$ that depends in a complicated way on the global error in the position coordinates q and vanishes on initialization [12]. The Kronecker product $(\mathbf{T}_+^{-1}\mathbf{T}_0) \otimes \mathbf{I}_m$ is composed of matrices

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

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

and the identity matrix $\mathbf{I}_m$. For algorithmic parameters α_m, α_f, β and γ according to Chung and Hulbert [4], the spectral radius of the iteration matrix in Eq. (8) is given by $\rho(\mathbf{T}_+^{-1}\mathbf{T}_0) = \rho_\infty$ 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 Eqs. (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 $h\mathbf{B}\big(q(t)\big)\mathbf{r}\big(t\big)$, see Eq. (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 Ref. [12].

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 $((\mathbf{T}_+^{-1}\mathbf{T}_0)^{n-n^*} \otimes \mathbf{I}_m)\mathbf{E}_{n^*}$ 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 Ref. [12], we get the error bound $\|\boldsymbol{\lambda}(t_n) - \boldsymbol{\lambda}_n\| \leq C(\bar{n}_\infty^2 \rho_\infty^{\bar{n}} h + h^2)$ with $\bar{n} := n - n^* \geq 0$ and a suitable constant $C > 0$.

4. 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.

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Appendix

A.1 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 Ref. [2], we consider a top rotating about a fixed point. In this appendix, we follow the presentation of the heavy top benchmark problem in Ref. [12, Sec. 5] using model parameters from Ref. [17, Sec. 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

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

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

$$\dot{\mathbf{x}} = \mathbf{u},\ \dot{\mathbf{R}} = \mathbf{R}\tilde{\boldsymbol{\Omega}} \tag{A.1a}$$

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

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

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

$$m\ddot{\mathbf{x}} - \boldsymbol{\lambda} = m\boldsymbol{\gamma}, \tag{A.1b}$$

$$\mathbf{J}\dot{\boldsymbol{\Omega}} + \boldsymbol{\Omega} \times \mathbf{J}\boldsymbol{\Omega} + \tilde{\mathbf{X}}\mathbf{R}^\top \boldsymbol{\lambda} = 0, \tag{A.1c}$$

$$-\mathbf{x} + \mathbf{R}\mathbf{X} = 0 \tag{A.1d}$$

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 Eq. (A.1d). 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

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

Omitting all physical units, the model data are given by $\mathbf{X} = (0, 1, 0)^\top$, $\boldsymbol{\gamma} = (0, 0, -9.81)^\top$, $m = 15$ and

$$\mathbf{J} = \mathrm{diag}(0.234375, 0.46875, 0.234375).$$

The (consistent) initial values are set to $\mathbf{x}(0) = \mathbf{X}$, $\mathbf{R}(0) = \mathbf{I}_3$, $\boldsymbol{\Omega}(0) = (0, 150, -4.61538)^\top$ and $\mathbf{u}(0) = -\tilde{\mathbf{X}}\boldsymbol{\Omega}(0)$.

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