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Abstract	Generalized- α methods are very popular in structural dynamics. They are methods of Newmark type and combine favourable stability properties with second order convergence for unconstrained second order systems in linear spaces. Recently, they were extended to constrained systems in flexible multibody dynamics that have a configuration space with Lie group structure. In the present paper, the convergence of these Lie group methods is analysed by a coupled one-step error recursion for differential and algebraic solution components. It is shown that spurious oscillations in the transient phase result from order reduction that may be avoided by a perturbation of starting values or by index reduction. Numerical tests for a benchmark problem from the literature illustrate the results of the theoretical investigations.

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Error analysis of generalized-α Lie group time integration methods for constrained mechanical systems

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Abstract Generalized-α methods are very popular in structural dynamics. They are methods of Newmark type and combine favourable stability properties with second order convergence for unconstrained second order systems in linear spaces. Recently, they were extended to constrained systems in flexible multibody dynamics that have a configuration space with Lie group structure. In the present paper, the convergence of these Lie group methods is analysed by a coupled one-step error recursion for differential and algebraic solution components. It is shown that spurious oscillations in the transient phase result from order reduction that may be avoided by a perturbation of starting values or by index reduction. Numerical tests for a benchmark problem from the literature illustrate the results of the theoretical investigations.

1 Introduction

In $\mathbb{R}^3$, the configuration of rigid body systems with large rotations can not be represented globally and free of singularities by elements of a linear space. Lie group formulations provide an alternative to avoid these singularities. They can characterize

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the rotational degrees of freedom for each body by a matrix of the rotation group SO(3) and result in nonlinear configuration spaces. This approach is not restricted to rigid body systems but has been used successfully as well in a finite element framework for the simulation of flexible multibody systems that is based on the set of nodal translations and rotations [19].

For time integration, Simo and Vu-Quoc proposed in 1988 a Newmark type method that exploits such Lie group structure of the configuration space directly and does not rely on local parametrizations of the Lie group [37]. Starting with the work of Crouch and Grossman [15] and Munthe-Kaas [31,32], the time integration of ordinary differential equations (ODEs) on Lie groups found later also much interest in the numerical analysis community, see the comprehensive review paper by Iserles et al. [23] and the compact summary in Chapter IV of the monograph by Hairer et al. [20].

In each time step of a Lie group method, elements of the Lie algebra are mapped to the Lie group resulting in a substantial numerical effort for evaluating exponential mappings, Cayley transforms or similar expressions [13,23]. Furthermore, the group action in the Lie group setting is in general not commutative and may result in a rapidly growing number of Lie brackets (in the case of matrix Lie groups: matrix commutators) that have to be evaluated to achieve high order in Lie group time integration [20,32,39].

The application to mechanical multibody systems has always been an important special case of Lie group time integration since the tensor product structure of the configuration space and the low dimension of its factors allow substantial savings of computing time in the evaluation of matrix exponentials and commutators, see, e.g., [7,13]. Moreover, the rather large numerical effort of high order Lie group time integration methods is not relevant in a method of lines approach to the simulation of flexible multibody systems since second order methods are sufficient to keep the time discretization error in the range of the errors resulting from the space discretization of flexible bodies by finite elements [19].

For these reasons, a new family of Lie group methods has recently been introduced that is tailored to the application in flexible multibody dynamics [9,10]. It is based on the generalized-α method for the time integration of unconstrained systems in linear spaces [14] that belongs to the class of Newmark type methods and exploits by construction the 2nd order structure of the equations of motion [34]. The generalized-α method is very popular in structural dynamics since it combines second order convergence with algorithmic damping of spurious high frequency oscillations resulting from the space discretization by finite elements [14,17,40].

For the application in multibody dynamics, the generalized-α method has to be extended to constrained systems with differential-algebraic equations of motion [19,21,40]. Following the classical approach of Cardona and Géradin [11], the method is applied directly to the index-3 formulation of the equations of motion [21] to support a straightforward implementation in existing finite element codes for unconstrained systems, see also [6] and the discussion of implementation aspects in industrial multibody system software in [33]. For the time integration in linear spaces, the combination of Newmark type methods with index reduction techniques for differential-algebraic equations (DAEs) has found much interest in the literature [2,24–26,29,40] but requires the additional evaluation of hidden constraints and the implementation of

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projection or stabilization techniques to avoid the drift-off effect [21] which might be non-trivial in an existing large scale simulation package.

There is one generalized-α method from the family of DAE Lie group time integration methods being proposed in [9] that proved to be especially attractive from the practical viewpoint. In the present paper, we analyse the convergence of this method in full detail. Considering local and global errors as elements of the corresponding Lie algebra [38], the convergence analysis of generalized-α methods for constrained systems in linear spaces [3] has recently been extended to the Lie group setting [4,10]. This analysis is based on an equivalent multi-step representation of the method [17] and proves second order convergence on finite time intervals. It is shown furthermore that the numerical results in long-term integration are not sensitive w.r.t. the definition of starting values since initial errors "are damped out rapidly" [3].

Numerical tests with time step sizes in the range of practical interest have shown, however, that initial errors may strongly be amplified in a transient phase [8]. This phenomenon was even observed for generalized-α methods with exact starting values for position and velocity coordinates and optimal algorithmic parameters α_m, α_f, β, γ according to Chung and Hulbert [14]. Moreover, the transient spurious oscillations were found as well in the application to constrained systems in linear spaces. This strange transient behaviour of generalized-α methods depends strongly on the choice of starting values and could not be analysed by our previous approach that relies on the equivalent multi-step representation according to Erlicher et al. [17], see [3,4,10].

Therefore, the convergence analysis in the present paper is strictly based on the original one-step formulation of the generalized-α method. For index-2 DAEs in linear spaces that result from mechanical systems with non-holonomic constraints, the analysis of Jay [24] shows that such one-step error recursions for Newmark type methods are on the one hand technically rather complicated but offer on the other hand deep insight in the convergence behaviour and provide the theoretical basis for developing variable time step size methods, see also [25].

For holonomic constraints and direct application of the Lie group generalized-α method to the index-3 formulation of the equations of motion, the analysis of the one-step error recursion results in a set of consistency and stability conditions for the algorithmic parameters α_m, α_f, β, γ that guarantee convergence with a global error being composed of a second order error term that dominates in long-term integration and a first order error term that may be amplified in a transient phase but is finally damped out by algorithmic damping.

For parameters α_m, α_f, β, γ that are optimal in the sense of Chung and Hulbert to achieve algorithmic damping with parameter $\rho_\infty \in [0, 1)$, see [14], the first order error terms in the starting values are amplified by powers of a 3×3 Jordan block with eigenvalue $\mu = -\rho_\infty$ that grow like $n^2|\mu|^n/2$. The first order error term may be eliminated perturbing the starting values for velocity and acceleration components. Alternatively, the generalized-α method could be applied to a Gear–Gupta–Leimkuhler like index reduced formulation of the equations of motion [4,18]. Here, the one-step error recursion shows second order convergence and the order reduction phenomenon does not appear.

The remaining part of the paper is organized as follows: In Sect. 2, we discuss the Lie group setting in more detail and introduce the generalized-α Lie group time

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integration method. Numerical test results for the simulation of the mathematical pendulum illustrate the spurious oscillations in the transient phase that are in the focus of interest of the present paper. The detailed convergence analysis in Sect. 3 is based on a coupled error recursion for differential and algebraic solution components and proves that the spurious oscillations in the transient phase result from order reduction. In Sect. 4, we discuss how to improve the transient behaviour by perturbed starting values or by index reduction. All results of the theoretical analysis are illustrated by simulation results for the Lie group representation of a rotating heavy top under the influence of gravity, see Sect. 5. The paper ends with a short summary and outlook in Sect. 6.

2 Lie group time integration by generalized-α methods

2.1 Lie group setting and equations of motion

The dynamics of flexible multibody systems with large rotations may be studied conveniently in a Lie group setting, see [19] and the more recent discussion in [9]. For this problem class, the equations of motion form a differential-algebraic equation

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

on a $k-m$ dimensional submanifold $\{q \in G \,:\, \boldsymbol{\Phi}(q) = \mathbf{0}\}$ of a k-dimensional manifold G with Lie group structure, see [20, Section IV.6] for a compact introduction to matrix Lie groups and for further references. As discussed in [9], the coordinates q may, e.g., represent the set of nodal translations and rotations in a finite element discretization of the flexible multibody system. It is important to observe that no local parametrization of the Lie group G is needed to formulate the equations of motion (1).

In this Lie group setting, the composition operation $G \times G \to G$ is denoted by $q_a \circ q_b \in G$ for any two elements $q_a, q_b \in G$. The configuration of the system is represented by $q \in G$ with a time derivative $\dot{q}(t)$ being determined by the velocity vector $\mathbf{v} \in \mathbb{R}^k$ in (1a). Here, the term $DL_q(e) \cdot \widetilde{\mathbf{v}}$ denotes the directional derivative of the left translation map $L_q \,:\, G \to G,\ y \mapsto q \circ y$ evaluated at the identity element $e \in G$ in direction $\widetilde{\mathbf{v}} \in \mathfrak{g}$. The map $DL_q(e)$ is a bijection between the Lie algebra $\mathfrak{g}$ of Lie group G and the tangent space T_qG of G at point $q \in G$. The Lie algebra $\mathfrak{g} := T_eG$ itself forms a linear space which is known to be isomorphic to $\mathbb{R}^k$ with an invertible linear mapping $\widetilde{(\bullet)} \,:\, \mathbb{R}^k \to \mathfrak{g},\ \mathbf{v} \mapsto \widetilde{\mathbf{v}}$.

The dynamic equations (1b) with the symmetric positive definite mass matrix $\mathbf{M} \in \mathbb{R}^{k\times k}$ and the vector $\mathbf{g}$ of external, internal and complementary inertia forces are coupled to the m constraints (1c) by Lagrange multipliers $\boldsymbol{\lambda} \in \mathbb{R}^m$ and by the matrix $\mathbf{B} \in \mathbb{R}^{m\times k}$ that represents the constraint gradients in the sense that

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

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with $D\mathbf{\Phi}(q)\cdot(DL_q(e)\cdot\widetilde{\mathbf{w}})$ denoting the directional derivative of $\mathbf{\Phi}\,:\,G\to\mathbb{R}^m$ evaluated at $q\in G$ in the direction $DL_q(e)\cdot\widetilde{\mathbf{w}}\in T_qG$.

Throughout the present paper, we suppose that $\mathbf{M}(q)$, $\mathbf{g}(q,\mathbf{v},t)$ and $\mathbf{\Phi}(q)$ are smooth in the sense that they are as often continuously differentiable as required by the convergence analysis.

Hidden constraints Holonomic constraints like (1c) restrict the set of consistent position coordinates $q\in G$ and imply so-called hidden constraints on velocity and acceleration variables that are given by time derivatives of $\mathbf{\Phi}(q(t))=\mathbf{0}$, see, e.g., [21]. Differentiating the constraints (1c) once, we obtain the hidden constraints on the level of velocity coordinates:

$$\mathbf{0}=\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{\Phi}(q(t))=D\mathbf{\Phi}(q(t))\cdot\dot q(t)=D\mathbf{\Phi}(q)\cdot\big(DL_q(e)\cdot\widetilde{\mathbf{v}}\big)=\mathbf{B}(q)\mathbf{v},\tag{3}$$

see (1a) and (2). A second differentiation of (1c) results in

$$\mathbf{0}=\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathbf{\Phi}(q(t))=\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{B}(q(t))\mathbf{v}(t)\right).$$

To express this time derivative in compact form, the vector valued function

$$\mathbf{\Theta}\,:\,G\times\mathbb{R}^k\to\mathbb{R}^m,\qquad\mathbf{\Theta}(q,\mathbf{z})=\mathbf{B}(q)\mathbf{z}\tag{4}$$

is introduced. Similar to the directional derivative of $\mathbf{\Phi}(q)$ that could be represented by the matrix valued function $\mathbf{B}$, there is a matrix valued function that represents the directional partial derivative of $\mathbf{\Theta}(q,\mathbf{z})$ with respect to $q\in G$. This matrix valued function is linear with respect to $\mathbf{z}\in\mathbb{R}^k$ since $\mathbf{\Theta}$ is linear with respect to $\mathbf{z}$ by construction. For any $\mathbf{z}\in\mathbb{R}^k$, we get

$$D_q\mathbf{\Theta}(q,\mathbf{z})\cdot\big(DL_q(e)\cdot\widetilde{\mathbf{w}}\big)=\mathbf{R}(q)(\mathbf{z},\mathbf{w}),\quad(\mathbf{w}\in\mathbb{R}^k)\tag{5}$$

with a bilinear form $\mathbf{R}(q)\,:\,\mathbb{R}^k\times\mathbb{R}^k\to\mathbb{R}^m$. The hidden constraints on the level of acceleration coordinates

$$\mathbf{0}=\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{B}(q(t))\mathbf{v}(t)\right)=\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{\Theta}\left(q(t),\mathbf{v}(t)\right)=\mathbf{B}(q)\dot{\mathbf{v}}+\mathbf{R}(q)\left(\mathbf{v},\mathbf{v}\right)\tag{6}$$

result from product and chain rule. A third differentiation of the holonomic constraints (1c) would result in a system of linear equations that could be solved for $\dot{\boldsymbol{\lambda}}(t)$ provided that matrix $\mathbf{B}(q)$ has full rank along the solution curve $q(t)$, see [21]. DAE (1) has differentiation index 3 and is called the *index-3 formulation* of the equations of motion.

Consistent initial values Initial values $q(t_0)$, $\mathbf{v}(t_0)$ for (1) have to be consistent with the (hidden) constraints (1c), (3), i.e., $\mathbf{\Phi}(q(t_0))=\mathbf{B}(q(t_0))\mathbf{v}(t_0)=\mathbf{0}$. Then, $\dot{\mathbf{v}}(t_0)$ and $\boldsymbol{\lambda}(t_0)$ are uniquely defined by the non-singular system of $k+m$ linear equations (1b), (6):

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$$\begin{pmatrix} \mathbf{M}_0 & \mathbf{B}_0^\top \\ \mathbf{B}_0 & \mathbf{0} \end{pmatrix} \begin{pmatrix} \dot{\mathbf{v}}(t_0) \\ \boldsymbol{\lambda}(t_0) \end{pmatrix} = \begin{pmatrix} -\mathbf{g}_0 \\ -\mathbf{R}_0 \end{pmatrix} \tag{7}$$

with $\mathbf{M}_0 := \mathbf{M}(q(t_0))$, etc.

2.2 Generalized-α methods for constrained systems on Lie groups

The time integration of (1) by generalized-α Lie group methods is based on the observation that (1a) implies

$$q(t+h) = q(t) \circ \exp\left(h\widetilde{\mathbf{v}}(t) + \frac{h^2}{2}\widetilde{\dot{\mathbf{v}}}(t) + \mathcal{O}(h^3) \right), \quad (h \to 0) \tag{8}$$

with the exponential map $\exp : \mathfrak{g} \to G$ that has the series expansion $\exp(\widetilde{\mathbf{w}}) = \sum_i \widetilde{\mathbf{w}}^i / i!$ for matrix Lie groups G and may be evaluated efficiently for typical applications in flexible multibody dynamics, see [8,9].

As proposed in [9], we consider a generalized-α method for the index-3 formulation (1) of the equations of motion that updates the numerical solution $(q_n, \mathbf{v}_n, \mathbf{a}_n, \boldsymbol{\lambda}_n)$ in a time step $t_n \to t_n + h$ of step size h according to

$$\begin{aligned} q_{n+1} &= q_n \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}_n), && \text{(9a)} \\ \boldsymbol{\Delta}\mathbf{q}_n &= \mathbf{v}_n + (0.5 - \beta)h\mathbf{a}_n + \beta h \mathbf{a}_{n+1}, && \text{(9b)} \\ \mathbf{v}_{n+1} &= \mathbf{v}_n + (1-\gamma)h\mathbf{a}_n + \gamma h \mathbf{a}_{n+1}, && \text{(9c)} \\ (1-\alpha_m)\mathbf{a}_{n+1} + \alpha_m \mathbf{a}_n &= (1-\alpha_f)\dot{\mathbf{v}}_{n+1} + \alpha_f \dot{\mathbf{v}}_n && \text{(9d)} \end{aligned}$$

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

$$\begin{aligned} \mathbf{M}(q_{n+1})\dot{\mathbf{v}}_{n+1} &= -\mathbf{g}(q_{n+1}, \mathbf{v}_{n+1}, t_{n+1}) - \mathbf{B}^\top(q_{n+1})\boldsymbol{\lambda}_{n+1}, && \text{(9e)} \\ \boldsymbol{\Phi}(q_{n+1}) &= \mathbf{0}. && \text{(9f)} \end{aligned}$$

The method is initialized by starting values q_0, $\mathbf{v}_0$, $\dot{\mathbf{v}}_0$ that are close to consistent initial values $q(t_0)$, $\mathbf{v}(t_0)$, $\dot{\mathbf{v}}(t_0)$, see (7), and by a starting value $\mathbf{a}_0 \approx \dot{\mathbf{v}}(t_0)$. A more sophisticated choice of starting values $\mathbf{v}_0$, $\mathbf{a}_0$ will be discussed in Sect. 4.2 below.

Method (9) is characterized by real parameters α_m, α_f, β and γ that are selected based on a linear stability analysis and on order conditions to guarantee second order convergence, see also [9,14]. In (9), the numerical solution $(q_{n+1}, \mathbf{v}_{n+1}, \mathbf{a}_{n+1}, \boldsymbol{\lambda}_{n+1})$ is implicitly defined by a system of nonlinear equations that may be solved by a Newton–Raphson iteration in terms of $(\boldsymbol{\Delta}\mathbf{q}_n^\top, \boldsymbol{\lambda}_{n+1}^\top)^\top \in \mathbb{R}^{k+m}$, see [10, Section 4]. For sufficiently small time step sizes $h > 0$ and any $q_n \in G$, $\mathbf{v}_n \in \mathbb{R}^k$ with $\boldsymbol{\Phi}(q_n) = \mathcal{O}(h^2)$, $\mathbf{B}(q_n)\mathbf{v}_n = \mathcal{O}(h)$, we may use ideas of the proof of Theorem VII.3.1 in [21] to show that (9) defines locally uniquely a vector $\boldsymbol{\Delta}\mathbf{q}_n \in \mathbb{R}^k$ with $\boldsymbol{\Delta}\mathbf{q}_n = \mathbf{v}_n + \mathcal{O}(h)$. Therefore, the argument $h\widetilde{\boldsymbol{\Delta}\mathbf{q}}_n = \mathcal{O}(h)$ of the exponential map in (9a) remains in a small neighbourhood of $\widetilde{\mathbf{0}} \in \mathfrak{g}$ on which exp is a diffeomorphism.

In the long-term simulation of conservative mechanical systems, Newmark type methods like (9) do not share the excellent nonlinear stability properties of variational

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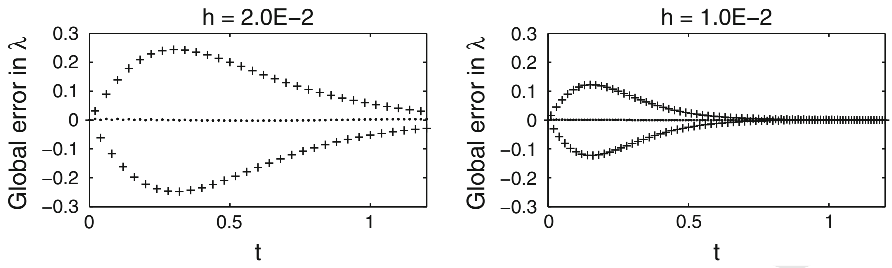

Fig. 1 Mathematical pendulum: Global error in λ for $x_0 = 0$ (...) and $x_0 = 0.2$ (+)

integrators [28] and of structure preserving algorithms in the sense of Simo and Tarnow [36], see also the detailed analysis of energy conservation in Newmark type methods for linear unconstrained systems in [27]. On the other hand, the collocation conditions (9e) allow a straightforward and efficient implementation of the generalized-α Lie group method in large scale simulation tools for flexible multibody systems with structural damping and other dissipative terms resulting, e.g., from friction or control structures. Furthermore, the method may be generalized directly to more complex model equations of constrained systems that are typical of industrial applications in multibody dynamics [2,5].

For kinematically excited systems (1) with time dependent constraints $\mathbf{\Phi}(q(t)) = \mathbf{c}(t)$, constraint (9f) is substituted by $\mathbf{\Phi}(q_{n+1}) = \mathbf{c}(t_{n+1})$. Moreover, the convergence analysis of the present paper may be extended to constrained systems with joint friction that are characterized by force vectors $\mathbf{g}$ in (1b) and (9e) depending on the constraint forces $-\mathbf{B}^\top(q)\boldsymbol{\lambda}$. To keep the presentation compact we omit the technical details of these more general investigations that require that matrix $\mathbf{BM}^{-1}((\partial\mathbf{g}/\partial\boldsymbol{\lambda}) + \mathbf{B}^\top)$ remains non-singular along the solution, see [2,5].

2.3 Spurious oscillations in the transient phase: example

Second order convergence of generalized-α methods for constrained systems (1) has been studied for several benchmark problems from mechanical engineering [8–10]. In [8], we observed in a transient phase spurious oscillations in $\boldsymbol{\lambda}$ that "are damped out rapidly" [3]. In the present section we study this problem in more detail for a simple test problem in a linear space, $G = \mathbb{R}^2$.

Example 1 Consider a mathematical pendulum of mass m and length l in Cartesian coordinates $q = (x, y)^\top$ that are constrained by $(x^2 + y^2 - l^2)/2 = 0$, see (1c). In (1), we have $\mathbf{M} = m\mathbf{I}_2$, $\mathbf{g} = (0, g)^\top$ with $m = l = 1$, $g = 9.81$ (physical units are omitted). We fix the total energy $E = m(\dot{x}_0^2 + \dot{y}_0^2)/2 + mgy_0$ to $E = m/2 - mgl$ and determine the consistent initial values x_0, y_0, $\dot{x}_0$, $\dot{y}_0$ and λ_0 by the initial deviation x_0 from the equilibrium position.

Method (9) is applied with parameters according to (52) and damping parameter $\rho_\infty = 0.9$, see [14]. Figure 1 shows on a short time interval the global error in λ for initial values $x_0 = 0$ (marked by dots) and $x_0 = 0.2$ (marked by "+") for two different step sizes h. If we start in the equilibrium position, the error is very small but for $x_0 = 0.2$, the oscillating error in λ reaches a maximum amplitude of 2.48×10^{-1} for $h = 2.0 \times 10^{-2}$ and 1.23×10^{-1} for $h = 1.0 \times 10^{-2}$. After about 100 time steps these transient errors are damped out.

The numerical results in Fig. 1 show that in the transient phase the generalized-α method (9) may suffer from spurious oscillations of amplitude $\mathcal{O}(h)$ which seems to contradict the second order convergence results in [3,10]. Spurious oscillations and order reduction disappear if we start at the equilibrium position $x_0 = 0$. Reducing the damping parameter ρ_∞ in (52), the oscillations are damped out more rapidly but may still be observed. The results are not sensitive to the definition of $\mathbf{a}_0$ that was in Fig. 1 set to $\mathbf{a}_0 = (\ddot{x}_0, \ \ddot{y}_0)^\top$. We repeated the numerical test for the less obvious but theoretically more favourable setting $\mathbf{a}_0 = (\ddot{x}(t_0 + \Delta_\alpha h), \ \ddot{y}(t_0 + \Delta_\alpha h))^\top + \mathcal{O}(h^2)$, see [25] and Lemma 1 below, and obtained up to plot accuracy identical results.

3 Convergence analysis

The convergence analysis of the generalized-α Lie group method (9) in our recent work [10] was guided by the convergence analysis of the (classical) generalized-α method for index-3 DAEs in linear spaces, see [3], that uses an equivalent multi-step representation according to Erlicher et al. [17]. As proposed by Wensch [38], the Lie group structure of the configuration space in (1) was addressed considering the errors in components $q \in G$ as elements of the Lie algebra $\mathfrak{g}$.

The multi-step representation allows a compact proof of second order convergence that ignores, however, the precise influence of starting values q_0, $\mathbf{v}_0$, $\dot{\mathbf{v}}_0$, $\mathbf{a}_0$ on the transient behaviour [3,10,17]. Therefore, we develop in the present section a pure one-step error recursion for (9) resulting in a convergence theorem that highlights the source of spurious oscillations and order reduction in the transient phase and shows how to fix these problems by modified starting values $\mathbf{v}_0$, $\mathbf{a}_0$, see Sect. 4.2. It explains furthermore, why the spurious oscillations may disappear for certain initial values, see Example 1, and for alternative Lie group settings [8].

3.1 Local and global errors

Local truncation error The convergence analysis will show that the numerical solution q_n, $\mathbf{v}_n$, $\mathbf{a}_n$, $\dot{\mathbf{v}}_n$, $\boldsymbol{\lambda}_n$ approximates $q(t_n)$, $\mathbf{v}(t_n)$, $\dot{\mathbf{v}}(t_n + \Delta_\alpha h)$, $\dot{\mathbf{v}}(t_n)$, $\boldsymbol{\lambda}(t_n)$ with $t_n = nh$ and a shift parameter $\Delta_\alpha \in \mathbb{R}$ that will be fixed in Lemma 1 below. Inserting these function values in (9), we get non-vanishing residuals $\mathbf{l}_n^{(\bullet)}$ (*local truncation errors*) in (9a,c,d):

$$q(t_{n+1}) = q(t_n) \circ \exp(h\widetilde{\mathbf{\Delta q}}(t_n)) \circ \exp(\widetilde{\mathbf{l}}_n^q), \tag{10a}$$

$$\mathbf{\Delta q}(t_n) = \mathbf{v}(t_n) + (0.5 - \beta)h\dot{\mathbf{v}}(t_n + \Delta_\alpha h) + \beta h\dot{\mathbf{v}}(t_{n+1} + \Delta_\alpha h), \tag{10b}$$

$$\mathbf{v}(t_{n+1}) = \mathbf{v}(t_n) + (1 - \gamma)h\dot{\mathbf{v}}(t_n + \Delta_\alpha h) + \gamma h\dot{\mathbf{v}}(t_{n+1} + \Delta_\alpha h) + \mathbf{l}_n^{\mathbf{v}}, \tag{10c}$$

$$(1 - \alpha_m)\dot{\mathbf{v}}(t_{n+1} + \Delta_\alpha h) + \alpha_m\dot{\mathbf{v}}(t_n + \Delta_\alpha h) = (1 - \alpha_f)\dot{\mathbf{v}}(t_{n+1}) + \alpha_f\dot{\mathbf{v}}(t_n) + \mathbf{l}_n^{\mathbf{a}}. \tag{10d}$$

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In (10a), we followed the approach of Wensch [38] who studied local and global errors of Lie group integrators for first order ordinary differential equations in the corresponding Lie algebra $\mathfrak{g}$. Lemma 1 below shows that (10a, b) defines for sufficiently small time step sizes $h > 0$ a locally unique local truncation error $\widetilde{\mathbf{l}}_n^q \in \mathfrak{g}$ with $\mathbf{l}_n^q = \mathcal{O}(h^3)$ since $q(t_n) \circ \exp(h\widetilde{\mathbf{\Delta q}}(t_n)) \in G$ coincides up to terms of size $\mathcal{O}(h^3)$ with $q(t_{n+1}) \in G$ and the exponential map exp is a diffeomorphism between neighbourhoods of $\widetilde{\mathbf{0}} \in \mathfrak{g}$ and $e \in G$.

Lemma 1 *With $\Delta_\alpha := \alpha_m - \alpha_f$, the local truncation errors are bounded by*

$$\|\mathbf{l}_n^q\| = \mathcal{O}(h^3), \quad \frac{1}{h}\|\mathbf{l}_{n+1}^q - \mathbf{l}_n^q\| = \mathcal{O}(h^3), \quad \|\mathbf{l}_n^{\mathbf{v}}\| = \mathcal{O}(h^3), \quad \|\mathbf{l}_n^{\mathbf{a}}\| = \mathcal{O}(h^2) \tag{11}$$

if the parameters γ, α_m, α_f satisfy the order condition

$$\gamma = \frac{1}{2} - \Delta_\alpha = \frac{1}{2} + \alpha_f - \alpha_m. \tag{12}$$

Proof The estimates for $\mathbf{l}_n^{\mathbf{v}}$, $\mathbf{l}_n^{\mathbf{a}}$ follow straightforwardly by Taylor expansion of $\mathbf{v}(t)$, $\dot{\mathbf{v}}(t)$ at $t = t_n$. To estimate $\mathbf{l}_n^q$, we consider the flow of $\dot{q}(t) = DL_q(e) \cdot \widetilde{\mathbf{v}}(t)$ that is locally represented by a smooth function $\widetilde{\boldsymbol{\nu}} : [-h_0, h_0] \times \mathbb{R} \times G \to \mathfrak{g}$ with an appropriate constant $h_0 > 0$ and $\boldsymbol{\nu}(0; t, q(t)) = \mathbf{v}(t)$, $(t \in \mathbb{R})$:

$$q(t+h) = q(t) \circ \exp\left(h\widetilde{\boldsymbol{\nu}}(h; t, q(t))\right). \tag{13}$$

For a given smooth function $\mathbf{v}(t)$, the Magnus expansion [20], see also [30], of $h\widetilde{\boldsymbol{\nu}}$ is given by

$$h\widetilde{\boldsymbol{\nu}}(h; t, q(t)) = h\widetilde{\mathbf{v}}(t) + \frac{h^2}{2}\dot{\widetilde{\mathbf{v}}}(t) + \frac{h^3}{6}\ddot{\widetilde{\mathbf{v}}}(t) + \frac{h^3}{12}[\widetilde{\mathbf{v}}(t), \dot{\widetilde{\mathbf{v}}}(t)] + \mathcal{O}(h^4) \tag{14}$$

with the commutator $[\mathbf{A}, \mathbf{C}] := \mathbf{AC} - \mathbf{CA}$ that vanishes identically in linear spaces but introduces an additional error term in the Lie group integrator whenever $\widetilde{\mathbf{v}}(t)$ and $\dot{\widetilde{\mathbf{v}}}(t)$ do not commute. With $q(t_{n+1}) = q(t_n + h)$, we obtain from (10a) and (13)

$$q(t_n) \circ \exp\left(h\widetilde{\boldsymbol{\nu}}(h; t_n, q(t_n))\right) = q(t_n) \circ \exp(h\widetilde{\mathbf{\Delta q}}(t_n)) \circ \exp(\widetilde{\mathbf{l}}_n^q),$$

$$\exp(\widetilde{\mathbf{l}}_n^q) = \exp(-h\widetilde{\mathbf{\Delta q}}(t_n)) \circ \exp(h\widetilde{\boldsymbol{\nu}}(h; t_n, q(t_n))). \tag{15}$$

This product of matrix exponentials is studied by the Baker–Campbell–Hausdorff formula that results in

$$\exp(\mathbf{A}) \circ \exp(\mathbf{C}) = \exp\left(\mathbf{A} + \mathbf{C} + \frac{1}{2}[\mathbf{A}, \mathbf{C}] + \mathcal{O}(h)\|[\mathbf{A}, \mathbf{C}]\|\right) \tag{16}$$

for matrices $\mathbf{A}$, $\mathbf{C}$ with $\mathbf{A} = \mathcal{O}(h)$, $\mathbf{C} = \mathcal{O}(h)$, see [20, Section III.4.2]. With $\mathbf{A} := -h\widetilde{\mathbf{\Delta q}}(t_n)$ and $\mathbf{C} := h\widetilde{\boldsymbol{\nu}}(h; t_n, q(t_n))$, the local truncation error $\widetilde{\mathbf{l}}_n^q$ in (10a) may be estimated by

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$$\begin{aligned}\widetilde{\mathbf{l}}_n^q &= h\widetilde{\boldsymbol{\nu}}(h;t_n,q(t_n)) - h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n) + \mathcal{O}(h)\|h\widetilde{\boldsymbol{\nu}}(h;t_n,q(t_n)) - h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)\| \\ &= \frac{h^3}{6}\left(\big(1-6\beta-3(\alpha_m-\alpha_f)\big)\,\dddot{\widetilde{\mathbf{v}}}(t_n) + \frac{1}{2}[\widetilde{\mathbf{v}}(t_n),\dot{\widetilde{\mathbf{v}}}(t_n)]\right) + \mathcal{O}(h^4) \qquad (17)\end{aligned}$$

since $[\mathbf{A},\mathbf{C}] = [\mathbf{A}+\mathbf{C},\mathbf{C}] - [\mathbf{C},\mathbf{C}] = \mathcal{O}(h)\|\mathbf{A}+\mathbf{C}\|$ if $\mathbf{C} = \mathcal{O}(h)$. This local truncation error $\widetilde{\mathbf{l}}_n^q = \mathcal{O}(h^3)$ varies smoothly in the sense that the leading error terms of $\widetilde{\mathbf{l}}_n^q$ and $\widetilde{\mathbf{l}}_{n+1}^q$ coincide up to $\mathcal{O}(h^4)$ and $\|\widetilde{\mathbf{l}}_{n+1}^q - \widetilde{\mathbf{l}}_n^q\|/h = \mathcal{O}(h^3)$. □

Global errors As for the local truncation error, the global error in components $q \in G$ is defined by an element of the Lie algebra:

$$q(t_n) = q_n \circ \exp(\widetilde{\mathbf{e}}_n^q), \qquad (18)$$

see [38]. Here, we assume implicitly that the numerical solution q_n is in a small neighbourhood of the analytical solution $q(t)$ at $t = t_n$ such that $\widetilde{\mathbf{e}}_n^q \in \mathfrak{g}$ is uniquely defined in a neighbourhood of $\widetilde{\mathbf{0}} \in \mathfrak{g}$ on which exp is a diffeomorphism, see also the more detailed discussion of the technical assumption (19) below. For solution components $\mathbf{v}(t)$, $\dot{\mathbf{v}}(t)$ and $\boldsymbol{\lambda}(t)$, that are elements of linear spaces, the global errors $\mathbf{e}_n^{(\bullet)}$ are defined by $(\bullet)(t_n) = (\bullet)_n + \mathbf{e}_n^{(\bullet)}$. In a similar way, the notation $\mathbf{e}_n^{\mathbf{a}}$ with $\dot{\mathbf{v}}(t_n + \Delta_\alpha h) = \mathbf{a}_n + \mathbf{e}_n^{\mathbf{a}}$ is introduced for the error in the numerical solution vector $\mathbf{a}_n$.

In the convergence analysis, we consider the equations of motion (1) on a finite time interval $[t_0, t_{\text{end}}]$ and assume that the numerical solution always remains in a small neighbourhood of the analytical one. More precisely, we suppose that there are positive constants h_0 and C and a sufficiently small constant $\gamma_0 > 0$ such that

$$\|\mathbf{e}_m^q\| \le Ch, \quad \|\mathbf{e}_m^{\mathbf{v}}\| + \|\mathbf{e}_m^{\mathbf{a}}\| + \|\mathbf{e}_m^{\boldsymbol{\lambda}}\| \le \gamma_0 \qquad (19)$$

is satisfied for all $h \in (0, h_0]$ and all m with $t_0 + mh \in [t_0, t_{\text{end}}]$. With this technical assumption, we will prove error bounds of size $\mathcal{O}(h^{1+\varepsilon}) + \mathcal{O}(h^2)$ with some $\varepsilon > 0$ for components q and $\mathbf{v}$ and of size $\mathcal{O}(h)$ for components $\boldsymbol{\lambda}$, $\dot{\mathbf{v}}$ and $\mathbf{a}$, see Theorem 1 below. Using this convergence result, assumption (19) with an appropriate (small) constant $h_0 > 0$ may finally be verified by induction whenever the assumptions of Theorem 1 are satisfied, see, e.g., part (c) of the proof of Theorem VII.3.5 in [21] for a detailed discussion.

3.2 One-step error recursion: differential components

The one-step error recursion is derived separately for the differential solution components q, $\mathbf{v}$ and the algebraic ones, see also Sect. 3.5 below. Because of the nonlinear Lie group structure, the error analysis for components $q \in G$ is technically more complicated than the one for components $\mathbf{v} \in \mathbb{R}^k$:

Lemma 2 *If the order condition* (12) *is satisfied then*

$$\mathbf{e}_{n+1}^q = \mathbf{e}_n^q + \mathcal{O}(h)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|) + \mathcal{O}(h^3), \qquad (20)$$

$$\mathbf{e}_{n+1}^{\mathbf{v}} = \mathbf{e}_n^{\mathbf{v}} + (1-\gamma)h\mathbf{e}_n^{\mathbf{a}} + \gamma h\mathbf{e}_{n+1}^{\mathbf{a}} + \mathcal{O}(h^3) \qquad (21)$$

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with the notation

$$\varepsilon_n := \|\mathbf{e}_n^q\| + \|\mathbf{e}_n^{\mathbf{v}}\| + h\|\mathbf{e}_n^{\mathbf{a}}\| + h\|\mathbf{e}_n^{\boldsymbol{\lambda}}\| \tag{22}$$

that allows to summarize higher order error terms in $h\varepsilon_n$. Furthermore, the scaled increment of global errors $\mathbf{e}_n^q$ is bounded by

$$\begin{aligned}\Delta_h \widetilde{\mathbf{e}}_n^q := \frac{\widetilde{\mathbf{e}}_{n+1}^q - \widetilde{\mathbf{e}}_n^q}{h} &= \widetilde{\mathbf{e}}_n^{\mathbf{v}} + (0.5-\beta)h\widetilde{\mathbf{e}}_n^{\mathbf{a}} + \beta h \widetilde{\mathbf{e}}_{n+1}^{\mathbf{a}} + [\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)] \\ &+ \mathcal{O}(h)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|) + \frac{1}{h}\widetilde{\mathbf{l}}_n^q. \end{aligned} \tag{23}$$

Proof Definition (18) implies $\exp(\widetilde{\mathbf{e}}_{n+1}^q) = (q_{n+1})^{-1} \circ q(t_{n+1})$. Therefore, we observe similar to the analysis in [10,35]

$$\begin{aligned}\exp(\widetilde{\mathbf{e}}_{n+1}^q) &= \exp(-h\widetilde{\boldsymbol{\Delta}\mathbf{q}}_n) \circ (q_n)^{-1} \circ q(t_n) \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)) \circ \exp(\widetilde{\mathbf{l}}_n^q), \\ &= \exp\left(h\widetilde{\mathbf{e}}_n^{\boldsymbol{\Delta}\mathbf{q}} - h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)\right) \circ \exp(\widetilde{\mathbf{e}}_n^q) \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)) \circ \exp(\widetilde{\mathbf{l}}_n^q|)\end{aligned}$$

with $\mathbf{e}_n^{\boldsymbol{\Delta}\mathbf{q}} := \boldsymbol{\Delta}\mathbf{q}(t_n) - \boldsymbol{\Delta}\mathbf{q}_n = \mathbf{e}_n^{\mathbf{v}} + (0.5-\beta)h\mathbf{e}_n^{\mathbf{a}} + \beta h\mathbf{e}_{n+1}^{\mathbf{a}}$. As in the proof of Lemma 1, the product of exponentials is studied by the Baker–Campbell–Hausdorff formula and (16). For matrices $\mathbf{A} = h\widetilde{\mathbf{e}}_n^{\boldsymbol{\Delta}\mathbf{q}} - h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n) = -h\widetilde{\mathbf{v}}(t_n) + \mathcal{O}(h)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|) + \mathcal{O}(h^2)$ and $\mathbf{C} = \widetilde{\mathbf{e}}_n^q = \mathcal{O}(h)$, see (19), we get

$$\exp(\mathbf{A}) \circ \exp(\mathbf{C}) = \exp\left(\mathbf{A} + \mathbf{C} + \frac{h}{2}[\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)] + \mathcal{O}(h^2)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|)\right)$$

since $[-\widetilde{\mathbf{v}}(t_n), \widetilde{\mathbf{e}}_n^q] = [\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)]$. Another $h/2 * [\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)]$ term results from the composition of $\exp(\mathbf{A} + \mathbf{C} + \ldots)$ with $\exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n))$. Finally, we obtain

$$\exp(\widetilde{\mathbf{e}}_{n+1}^q) = \exp\left(\widetilde{\mathbf{e}}_n^q + h\widetilde{\mathbf{e}}_n^{\boldsymbol{\Delta}\mathbf{q}} + h[\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)] + \widetilde{\mathbf{l}}_n^q + \mathcal{O}(h^2)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|)\right). \tag{24}$$

Since the arguments of the exponentials on both sides of (24) coincide, estimates (20) and (23) follow straightforwardly from (24) and $\|\mathbf{l}_n^q\| = \mathcal{O}(h^3)$.

Estimate (21) for the global error $\mathbf{e}_n^{\mathbf{v}}$ results from the difference of (10c) and (9c) taking into account $\|\mathbf{l}_n^{\mathbf{v}}\| = \mathcal{O}(h^3)$, see also Lemma 1. □

3.3 Error estimates for algebraic components

Error bounds for $\dot{\mathbf{v}}$ are obtained from the equilibrium conditions (1b), (9e) that are satisfied both for the analytical and for the numerical solution.

Lemma 3 *If the order condition* (12) *is satisfied then*

$$\mathbf{e}_n^{\dot{\mathbf{v}}} + \mathbf{e}_n^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}} = \mathcal{O}(1)\varepsilon_n, \quad \|\mathbf{e}_n^{\dot{\mathbf{v}}}\| = \mathcal{O}(1)(\varepsilon_n + \|\mathbf{e}_n^{\boldsymbol{\lambda}}\|), \tag{25a}$$

$$\mathbf{e}_{n+1}^{\dot{\mathbf{v}}} + \mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}} = \mathcal{O}(1)\varepsilon_n + \mathcal{O}(h)(\|\mathbf{e}_{n+1}^{\mathbf{a}}\| + \|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\|) + \mathcal{O}(h^3). \tag{25b}$$

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Here we used the notation $\mathbf{e}_n^{(\mathbf{C}\,\bullet)} := \mathbf{C}(q(t_n), \mathbf{v}(t_n), \boldsymbol{\lambda}(t_n), t_n)\mathbf{e}_n^{(\bullet)}$ *for matrix valued functions* $\mathbf{C} = \mathbf{C}(q, \mathbf{v}, \boldsymbol{\lambda}, t)$.

Proof To prove (25a), the equilibrium conditions (1b), (9e) at $t = t_n$ are multiplied by $\mathbf{M}^{-1}(q(t_n))$ and $\mathbf{M}^{-1}(q_n)$, respectively. For the error bound (25b) at $t = t_{n+1}$, the global errors $\|\mathbf{e}_{n+1}^q\|$, $\|\mathbf{e}_{n+1}^{\mathbf{v}}\|$ are substituted by the estimates (20), (21) from Lemma 2. □

Remark 1 With slightly stronger assumptions, Lemma 3 may be generalized to constrained systems with joint friction resulting in a force vector that depends on the constraint forces $-\mathbf{B}^\top(q)\boldsymbol{\lambda}$. In that case, we have $\mathbf{g} = \mathbf{g}(q, \mathbf{v}, \boldsymbol{\lambda}, t)$ and matrix $\mathbf{B}^\top$ in $\mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}}$ is replaced by $(\partial\mathbf{g}/\partial\boldsymbol{\lambda}) + \mathbf{B}^\top$. To make sure that the argument of $\partial\mathbf{g}/\partial\boldsymbol{\lambda}$ remains in an $\mathcal{O}(h)$-neighbourhood of the analytical solution, constant γ_0 in (19) has to be substituted by Ch whenever $\partial\mathbf{g}/\partial\boldsymbol{\lambda} \neq \mathbf{0}$. This sharper technical assumption may again be verified by standard arguments if the non-negative constant δ in Theorem 1 satisfies $\delta > 0$.

3.4 Time discrete approximations of (hidden) constraints

In linear spaces, the key to the convergence analysis of algebraic components in the time integration of higher index DAEs are difference approximations of (hidden) constraints combined with appropriate bounds for the approximation errors, see, e.g., [3]. Similar time discrete approximations of original and hidden constraints may be obtained in the Lie group setting. They allow to estimate products of the constraint matrix $\mathbf{B}(q)$ with error terms $\mathbf{e}_n^q$ and $\boldsymbol{\Delta}_h\mathbf{e}_n^q$:

Lemma 4 *The global errors* $\mathbf{e}_n^q \in \mathbb{R}^k$ *satisfy*

$$-\mathbf{D}_{0,n} = \mathbf{B}\left(q(t_n)\right)\mathbf{e}_n^q + \mathcal{O}(h)\|\mathbf{e}_n^q\|, \tag{26}$$

$$-\mathbf{D}_{1,n} = \mathbf{B}\left(q(t_n)\right)\boldsymbol{\Delta}_h\mathbf{e}_n^q + \mathbf{R}\left(q(t_n)\right)\left(\mathbf{e}_n^q, \mathbf{v}(t_n)\right) + \mathcal{O}(h)(\|\mathbf{e}_n^q\| + \|\boldsymbol{\Delta}_h\mathbf{e}_n^q\|) \tag{27}$$

with

$$\mathbf{D}_{0,n} := \boldsymbol{\Phi}(q_n), \quad \mathbf{D}_{k+1,n} := \frac{\mathbf{D}_{k,n+1} - \mathbf{D}_{k,n}}{h}, \ (k \geq 0). \tag{28}$$

Note, that formally $\mathbf{D}_{k,n} = \mathbf{0}$, *see* (9f), *but in a practical implementation there may be small residuals that result from stopping the corrector iteration after a finite number of Newton steps and from round-off errors.*

Proof For $\vartheta \in [0, 1]$, we define $q_{n,\vartheta} := q(t_n) \circ \exp(-\vartheta\widetilde{\mathbf{e}}_n^q) \in G$ such that $q_{n,0} = q(t_n)$, $q_{n,1} = q_n$ and get

$$-\frac{\mathrm{d}}{\mathrm{d}\vartheta}\boldsymbol{\Phi}(q_{n,\vartheta}) = \mathbf{B}(q_{n,\vartheta})\mathbf{e}_n^q = \mathbf{B}\left(q(t_n)\right)\mathbf{e}_n^q + \mathcal{O}(h)\|\mathbf{e}_n^q\|,$$

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see (2). Assertion (26) follows from $\mathbf{\Phi}(q_{n,1}) = \mathbf{\Phi}(q_n)$, $\mathbf{\Phi}(q_{n,0}) = \mathbf{\Phi}(q(t_n)) = \mathbf{0}$ and

$$-\mathbf{D}_{0,n} = -\mathbf{\Phi}(q_n) = -\big(\mathbf{\Phi}(q_{n,1}) - \mathbf{\Phi}(q_{n,0})\big) = \int_0^1 \mathbf{B}(q_{n,\vartheta})\mathbf{e}_n^q \,\mathrm{d}\vartheta. \qquad (29)$$

To prove assertion (27), we introduce the notation $q_{n+\sigma,\vartheta} := q_{n,\vartheta} \circ \exp(\sigma\widetilde{\mathbf{e}}_{n,\vartheta})$, $(\sigma \in [0,1])$, with $\widetilde{\mathbf{e}}_{n,\vartheta} \in \mathfrak{g}$ being implicitly defined by $q_{n+1,\vartheta} = q_{n,\vartheta} \circ \exp(\widetilde{\mathbf{e}}_{n,\vartheta})$. Scaling the difference of (29) for $t = t_{n+1}$ and $t = t_n$ by $1/h$, we get

$$-\mathbf{D}_{1,n} = \int_0^1 \mathbf{B}(q_{n+1,\vartheta})\mathbf{\Delta}_h\mathbf{e}_n^q \,\mathrm{d}\vartheta + \frac{1}{h}\int_0^1 \big(\mathbf{B}(q_{n+1,\vartheta}) - \mathbf{B}(q_{n,\vartheta})\big)\,\mathbf{e}_n^q \,\mathrm{d}\vartheta. \qquad (30)$$

The second integrand may be transformed using the bilinear form $\mathbf{R}$, see (5):

$$\begin{aligned}\big(\mathbf{B}(q_{n+1,\vartheta}) - \mathbf{B}(q_{n,\vartheta})\big)\,\mathbf{e}_n^q &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\sigma}\big(\mathbf{B}(q_{n+\sigma,\vartheta})\mathbf{e}_n^q\big)\,\mathrm{d}\sigma \\ &= \int_0^1 \mathbf{R}(q_{n+\sigma,\vartheta})\big(\mathbf{e}_n^q, \mathbf{e}_{n,\vartheta}\big)\,\mathrm{d}\sigma. \qquad (31)\end{aligned}$$

To complete the proof of (27), we show now the estimate

$$\mathbf{e}_{n,\vartheta} = h\mathbf{v}(t_n) + \mathcal{O}(h)\|\mathbf{\Delta}_h\mathbf{e}_n^q\| + \mathcal{O}(h^2) \qquad (32)$$

that allows to substitute the integrand $\mathbf{R}(q_{n+\sigma,\vartheta})(\mathbf{e}_n^q, \mathbf{e}_{n,\vartheta})$ in (31) by

$$h\mathbf{R}(q(t_n))\big(\mathbf{e}_n^q, \mathbf{v}(t_n)\big) + \mathcal{O}(h^2)(\|\mathbf{e}_n^q\| + \|\mathbf{\Delta}_h\mathbf{e}_n^q\|).$$

To prove (32), we represent $\exp(\widetilde{\mathbf{e}}_{n,\vartheta})$ as product of matrix exponentials:

$$\begin{aligned}\exp(\widetilde{\mathbf{e}}_{n,\vartheta}) = (q_{n,\vartheta})^{-1} \circ q_{n+1,\vartheta} &= \exp(\vartheta\widetilde{\mathbf{e}}_n^q) \circ (q(t_n))^{-1} \circ q(t_{n+1}) \circ \exp(-\vartheta\widetilde{\mathbf{e}}_{n+1}^q) \\ &= \exp(\vartheta\widetilde{\mathbf{e}}_n^q) \circ \exp\Big(h\widetilde{\mathbf{v}}(t_n) + \mathcal{O}(h^2)\Big) \circ \exp(-\vartheta\widetilde{\mathbf{e}}_n^q - h\vartheta\,\mathbf{\Delta}_h\widetilde{\mathbf{e}}_n^q),\end{aligned}$$

see (8). Estimate (32) follows from repeated application of the Baker–Campbell–Hausdorff formula taking into account $\|\mathbf{e}_n^q\| = \mathcal{O}(h)$, see (19). □

Corollary 1 *Consider a method* (9) *with* (12), $\alpha_m \neq 1$, $\alpha_f \neq 1$ *and* $\beta \neq 0$.

(a) *The scaled global errors in the algebraic components are bounded by*

$$h(\|\mathbf{e}_{n+1}^{\mathbf{a}}\| + \|\mathbf{e}_{n+1}^{\dot{\mathbf{v}}}\| + \|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\|) = \mathcal{O}(1)(\varepsilon_n + \|\mathbf{D}_{1,n}\|) + \mathcal{O}(h^2). \qquad (33)$$

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(b) *Let* $\mathbf{r}_n \in \mathbb{R}^k$ *be defined by*

$$h\mathbf{r}_n = \mathbf{\Delta}_h \mathbf{e}_n^q - (0.5 - \beta)h\mathbf{e}_n^{\mathbf{a}} - \beta h \mathbf{e}_{n+1}^{\mathbf{a}}. \tag{34}$$

The corresponding element $\widetilde{\mathbf{r}}_n \in \mathfrak{g}$ *satisfies*

$$h\widetilde{\mathbf{r}}_n = \widetilde{\mathbf{e}}_n^{\mathbf{v}} + [\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)] + \frac{1}{h}\widetilde{\mathbf{l}}_n^q + \mathcal{O}(h)(\varepsilon_n + \|\mathbf{D}_{1,n}\|) + \mathcal{O}(h^3). \tag{35}$$

Proof a) Multiplying the difference of (10d) and (9d) by h and substituting $h\mathbf{e}_{n+1}^{\dot{\mathbf{v}}}$ by $-h\mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}}$ and some higher order terms, see (25b), we get

$$(1-\alpha_m)h\mathbf{e}_{n+1}^{\mathbf{a}} + (1-\alpha_f)h\mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}} = \mathcal{O}(1)\varepsilon_n + \mathcal{O}(h^2)(\|\mathbf{e}_{n+1}^{\mathbf{a}}\| + \|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\|) + \mathcal{O}(h^3)$$

since $h\|\mathbf{l}_n^{\mathbf{a}}\| = \mathcal{O}(h^3)$, $h\|\mathbf{e}_n^{\mathbf{a}}\| \le \varepsilon_n$ and $h\|\mathbf{e}_n^{\dot{\mathbf{v}}}\|$ is bounded by (25a). Because of $\alpha_m \neq 1$, these equations may be solved w.r.t. $h\mathbf{e}_{n+1}^{\mathbf{a}}$ if $h > 0$ is sufficiently small:

$$h\mathbf{e}_{n+1}^{\mathbf{a}} = -\frac{1-\alpha_f}{1-\alpha_m}h\mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}} + \mathcal{O}(1)\varepsilon_n + \mathcal{O}(h^2)\|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\| + \mathcal{O}(h^3). \tag{36}$$

In (23), an estimate for $\mathbf{\Delta}_h\widetilde{\mathbf{e}}_n^q \in \mathfrak{g}$ in terms of $\widetilde{\mathbf{e}}_n^q$, $\widetilde{\mathbf{e}}_n^{\mathbf{v}}$, $h\widetilde{\mathbf{e}}_n^{\mathbf{a}}$ and $h\widetilde{\mathbf{e}}_{n+1}^{\mathbf{a}}$ is given. With (36), the equivalent estimate for $\mathbf{\Delta}_h\mathbf{e}_n^q \in \mathbb{R}^k$ may be transformed to

$$\mathbf{\Delta}_h\mathbf{e}_n^q = -\beta\frac{1-\alpha_f}{1-\alpha_m}h\mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}} + \mathcal{O}(1)\varepsilon_n + \mathcal{O}(h^2)\|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\| + \mathcal{O}(h^2)$$

since $\|\mathbf{e}_n^q\| + \|\mathbf{e}_n^{\mathbf{v}}\| + h\|\mathbf{e}_n^{\mathbf{a}}\| \le \varepsilon_n$ and $\|\mathbf{l}_n^q\|/h = \mathcal{O}(h^2)$. Substituting this expression in the time discrete approximation (27) of the hidden constraints at the level of acceleration variables, we get

$$-\mathbf{D}_{1,n} = -\beta\frac{1-\alpha_f}{1-\alpha_m}h\mathbf{e}_{n+1}^{\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}} + \mathcal{O}(1)\varepsilon_n + \mathcal{O}(h^2)\|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\| + \mathcal{O}(h^2).$$

The Implicit function theorem may be used to show that these equations are locally uniquely solvable w.r.t. $h\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}$ since the matrix product $\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top$ is non-singular for any full rank matrix $\mathbf{B}$ if mass matrix $\mathbf{M}$ is symmetric positive definite. This proves estimate (33) for $h\|\mathbf{e}_{n+1}^{\boldsymbol{\lambda}}\|$. The corresponding estimates for $h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|$ and $h\|\mathbf{e}_{n+1}^{\dot{\mathbf{v}}}\|$ are obtained from (36) and (25b), respectively.

(b) To prove (35), we use error bound (33) to substitute in (23) the higher order error term $\mathcal{O}(h)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|)$ by $\mathcal{O}(h)(\varepsilon_n + \|\mathbf{D}_{1,n}\|) + \mathcal{O}(h^3)$. □

Remark 2 The higher order error term $\mathcal{O}(h)(\varepsilon_n + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|)$ in (23) results from higher order terms in the Baker–Campbell–Hausdorff formula and vanishes identically for equations of motion (1) in linear spaces. In that case, estimate (35) gets the simpler form $h\mathbf{r}_n = \mathbf{e}_n^{\mathbf{v}} + \mathbf{l}_n^q/h = \mathbf{e}_n^{\mathbf{v}} + \mathcal{O}(h^2)$ and does *not* contain any global errors $\mathbf{e}_{n+1}^{(\bullet)}$, see (23).

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In the general Lie group setting of (1), the analysis of Corollary 1 is necessary to eliminate the $\mathcal{O}(h)(h\|\mathbf{e}^{\mathbf{a}}_{n+1}\|)$ error term from (23) since otherwise the difference $\mathbf{r}_{n+1} - \mathbf{r}_n$ in the one-step error recursion of algebraic solution components would depend on $h^2\|\mathbf{e}^{\mathbf{a}}_{n+2}\|$, see the proof of Lemma 6 below.

3.5 One-step error recursion: algebraic components

The difference of (10d) and (9d) connects the error propagation in the algebraic solution components $\mathbf{a}$ and $\dot{\mathbf{v}}$. With (25), the global errors $\mathbf{e}^{\dot{\mathbf{v}}}_n$ and $\mathbf{e}^{\dot{\mathbf{v}}}_{n+1}$ can be eliminated resulting in

$$\begin{aligned}&(1-\alpha_m)\mathbf{e}^{\mathbf{a}}_{n+1} + \alpha_m \mathbf{e}^{\mathbf{a}}_n + (1-\alpha_f)\mathbf{e}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}}_{n+1} + \alpha_f \mathbf{e}^{\mathbf{M}^{-1}\mathbf{B}^\top\boldsymbol{\lambda}}_n\\ &\quad = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(1)\|\mathbf{l}^{\mathbf{a}}_n\| \end{aligned} \tag{37}$$

To prove optimal error bounds, this coupled error recursion is studied separately in tangential and normal direction of the constraint manifold $\mathfrak{M} := \{q \in G \,:\, \boldsymbol{\Phi}(q) = \mathbf{0}\}$, see [21]. For any $q \in \mathfrak{M}$, the matrix

$$\mathbf{P}(q) := \mathbf{I} - [\mathbf{M}^{-1}\mathbf{B}^\top\mathbf{S}^{-1}\mathbf{B}](q) \;\text{ with }\; \mathbf{S}(q) := [\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^\top](q) \tag{38}$$

is a projector into the tangential space $T_q\mathfrak{M}$ since $\mathbf{BP} = \mathbf{B} - \mathbf{BM}^{-1}\mathbf{B}^\top\mathbf{S}^{-1}\mathbf{B} = \mathbf{B} - \mathbf{SS}^{-1}\mathbf{B} = \mathbf{0}$, $\mathbf{PP} = \mathbf{P}$ and $\ker \mathbf{B} = T_q\mathfrak{M}$.

Lemma 5 *The global errors $\mathbf{e}^{\mathbf{a}}_n$, $\mathbf{e}^{\boldsymbol{\lambda}}_n$ satisfy*

$$(1-\alpha_m)\mathbf{e}^{\mathbf{Pa}}_{n+1} + \alpha_m \mathbf{e}^{\mathbf{Pa}}_n = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2), \tag{39}$$

$$(1-\alpha_m)\mathbf{e}^{\mathbf{Ba}}_{n+1} + \alpha_m \mathbf{e}^{\mathbf{Ba}}_n + (1-\alpha_f)\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1} + \alpha_f \mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_n = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2) \tag{40}$$

and $\|\mathbf{e}^{\mathbf{a}}_n\| \le \|\mathbf{e}^{\mathbf{Pa}}_n\| + \|\mathbf{M}^{-1}\mathbf{B}^\top\mathbf{S}^{-1}\|\|\mathbf{e}^{\mathbf{Ba}}_n\| \le \mathcal{O}(1)(\|\mathbf{e}^{\mathbf{Pa}}_n\| + \|\mathbf{e}^{\mathbf{Ba}}_n\|)$.

Proof The errors in $\boldsymbol{\lambda}$ are bounded by $\|\mathbf{e}^{\boldsymbol{\lambda}}_n\| \le \mathcal{O}(1)\|\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_n\|$ since $\mathbf{S}$ is non-singular. Therefore, the lemma is a trivial consequence of (37) and $\mathbf{PM}^{-1}\mathbf{B}^\top \equiv \mathbf{0}$. Note, that $\|\mathbf{l}^{\mathbf{a}}_n\| = \mathcal{O}(h^2)$ for *any* parameter values α_m, α_f. □

Estimate (39) defines a one-step recursion for the tangential error component $\mathbf{e}^{\mathbf{Pa}}_n$ in terms of ε_n, ε_{n+1} and local errors $\mathcal{O}(h^2)$. To complete the error analysis, another recursive estimate is necessary for error component $\mathbf{e}^{\mathbf{Ba}}_n$.

This additional estimate will be obtained from the time discrete approximation (27) of the hidden constraints at the level of acceleration coordinates. For this purpose, we substitute in (27) the term $\mathbf{B}(q(t_n))\boldsymbol{\Delta}_h\mathbf{e}^q_n$ by $\mathbf{B}(q(t_n))\mathbf{r}_n$ with vector $\mathbf{r}_n$ from Corollary 1b, see (34), and use the notation

$$\mathbf{r}^{\mathbf{B}}_n := \mathbf{B}(q(t_n))\mathbf{r}_n + \frac{1}{h}\left(\mathbf{D}_{1,n} + \mathbf{R}(q(t_n))\left(\mathbf{e}^q_n, \mathbf{v}(t_n)\right)\right). \tag{41}$$

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Lemma 6 *Under the assumptions of Corollary 1 vectors* $\mathbf{r}_n^{\mathbf{B}}$ *satisfy*

$$\mathbf{r}_n^{\mathbf{B}} + (0.5-\beta)\mathbf{e}_n^{\mathbf{Ba}} + \beta\mathbf{e}_{n+1}^{\mathbf{Ba}} = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2), \tag{42}$$

$$\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}} = (1-\gamma)\mathbf{e}_n^{\mathbf{Ba}} + \gamma\mathbf{e}_{n+1}^{\mathbf{Ba}} + \mathbf{D}_{2,n} + \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1} + \|\mathbf{D}_{1,n}\| + h\|\mathbf{D}_{2,n}\|) + \mathcal{O}(h^2). \tag{43}$$

Proof Scaling the discrete approximation (27) of the hidden constraint by $1/h$, we get estimate (42) directly from the definition of $\mathbf{r}_n^{\mathbf{B}}$, see (34) and (41):

$$\begin{aligned}\mathbf{r}_n^{\mathbf{B}} + (0.5-\beta)\mathbf{e}_n^{\mathbf{Ba}} + \beta\mathbf{e}_{n+1}^{\mathbf{Ba}} &= \frac{\mathbf{B}(q(t_n))\boldsymbol{\Delta}_h\mathbf{e}_n^q + \mathbf{D}_{1,n} + \mathbf{R}(q(t_n))\left(\mathbf{e}_n^q, \mathbf{v}(t_n)\right)}{h} \\ &\quad + \mathcal{O}(h)\|\mathbf{e}_{n+1}^{\mathbf{a}}\| \\ &= \mathcal{O}(1)(\|\mathbf{e}_n^q\| + \|\boldsymbol{\Delta}_h\mathbf{e}_n^q\| + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|)\end{aligned}$$

with $\|\mathbf{e}_n^q\| \le \varepsilon_n, h\|\mathbf{e}_{n+1}^{\mathbf{a}}\| \le \varepsilon_{n+1}$ and $\|\boldsymbol{\Delta}_h\mathbf{e}_n^q\| = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)$, see (23).

For the proof of (43), the scaled differences $h(\widetilde{\mathbf{r}}_{n+1} - \widetilde{\mathbf{r}}_n)$ and $h(\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}})$ are studied term by term, see (35) and (41): The first term of the difference of (35) for $t = t_{n+1}$ and $t = t_n$ is $\widetilde{\mathbf{e}}_{n+1}^{\mathbf{v}} - \widetilde{\mathbf{e}}_n^{\mathbf{v}}$ and contributes to the difference $\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}}$ in (43) the term

$$\frac{\mathbf{e}_{n+1}^{\mathbf{Bv}} - \mathbf{e}_n^{\mathbf{Bv}}}{h} = (1-\gamma)\mathbf{e}_n^{\mathbf{Ba}} + \gamma\mathbf{e}_{n+1}^{\mathbf{Ba}} + \mathcal{O}(1)(\|\mathbf{e}_n^{\mathbf{v}}\| + h\|\mathbf{e}_n^{\mathbf{a}}\|) + \mathcal{O}(h^2),$$

with $\|\mathbf{e}_n^{\mathbf{v}}\| + h\|\mathbf{e}_n^{\mathbf{a}}\| \le \varepsilon_n$, see (21). The second term in $h(\widetilde{\mathbf{r}}_{n+1} - \widetilde{\mathbf{r}}_n)$ is

$$\begin{aligned}[\widetilde{\mathbf{e}}_{n+1}^q, \widetilde{\mathbf{v}}(t_{n+1})] - [\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)] &= [\widetilde{\mathbf{e}}_{n+1}^q, \widetilde{\mathbf{v}}(t_{n+1}) - \widetilde{\mathbf{v}}(t_n)] + h[\boldsymbol{\Delta}_h\widetilde{\mathbf{e}}_n^q, \widetilde{\mathbf{v}}(t_n)] \\ &= \mathcal{O}(h)(\|\mathbf{e}_{n+1}^q\| + \|\boldsymbol{\Delta}_h\mathbf{e}_n^q\|).\end{aligned}$$

It contributes to $\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}}$ a higher order term $\mathcal{O}(1)(\|\mathbf{e}_{n+1}^q\| + \|\boldsymbol{\Delta}_h\mathbf{e}_n^q\|)$ that is bounded by $\mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)$, see above. For the same reason, also the $\mathbf{R}(q(t_n))(\mathbf{e}_n^q, \mathbf{v}(t_n))$-term in (41) contributes only higher order terms of size $\mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2)$ to $\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}}$.

The third term in $h(\widetilde{\mathbf{r}}_{n+1} - \widetilde{\mathbf{r}}_n)$ is the scaled difference $(\widetilde{\mathbf{l}}_{n+1}^q - \widetilde{\mathbf{l}}_n^q)/h$ of local errors $\widetilde{\mathbf{l}}_n^q$ that is of size $\mathcal{O}(h^3)$ and contributes to $\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}}$ a local error term $\mathcal{O}(h^2)$, see Lemma 1. Note, that it is important to prove $\|\mathbf{l}_{n+1}^q - \mathbf{l}_n^q\| = \mathcal{O}(h^4)$ since the classical local error estimate $\|\mathbf{l}_n^q\| = \mathcal{O}(h^3)$ alone would not have been sufficient to prove estimate (43) with a bound of size $\mathcal{O}(h^2)$.

The remaining terms in $h(\widetilde{\mathbf{r}}_{n+1} - \widetilde{\mathbf{r}}_n)$ contribute higher order terms of size $\mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1} + \|\mathbf{D}_{1,n}\| + h\|\mathbf{D}_{2,n}\|) + \mathcal{O}(h^2)$ to $\mathbf{r}_{n+1}^{\mathbf{B}} - \mathbf{r}_n^{\mathbf{B}}$ since $\|\mathbf{D}_{1,n+1}\| \le \|\mathbf{D}_{1,n}\| + h\|\mathbf{D}_{2,n}\|$, see (28) and (35).

Finally, the $\mathbf{D}_{1,n}$-term in (41) yields the term $\mathbf{D}_{2,n}$ in the right hand side of (43). This completes the proof of estimate (43) and Lemma 6. □

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3.6 Synthesis

The coupled error propagation in differential and algebraic solution components is studied generalizing the convergence theory for one-step DAE time integration methods. With notations

$$\mathbf{E}^{\mathbf{r}}_n := \left((\mathbf{r}^{\mathbf{B}}_n)^\top,\ (\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_n)^\top,\ (\mathbf{e}^{\mathbf{Ba}}_n)^\top \right)^\top, \quad \theta := \max_{0 \le mh \le t_{\mathrm{end}} - t_0} \|\boldsymbol{\Phi}(q_m)\|, \tag{44}$$

estimates (42), (43) and (40) can be summarized in compact form:

$$\|(\mathbf{T}_+ \otimes \mathbf{I}_m)\mathbf{E}^{\mathbf{r}}_{n+1} - (\mathbf{T}_0 \otimes \mathbf{I}_m)\mathbf{E}^{\mathbf{r}}_n\| = \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^{-2})\theta + \mathcal{O}(h^2) \tag{45}$$

with the Kronecker product $\otimes$ and matrices

$$\mathbf{T}_+ = \begin{pmatrix} 0 & 0 & -\beta \\ 1 & 0 & -\gamma \\ 0 & 1-\alpha_f & 1-\alpha_m \end{pmatrix}, \quad \mathbf{T}_0 = \begin{pmatrix} 1 & 0 & 0.5-\beta \\ 1 & 0 & 1-\gamma \\ 0 & -\alpha_f & -\alpha_m \end{pmatrix} \tag{46}$$

that depend on the parameters of the generalized-α method (9). Note, that (45) is valid only if $t_{n+1} + h = t_n + 2h \le t_{\mathrm{end}}$ because of the term $\mathbf{D}_{2,n}$ in (43) that depends on $\mathbf{D}_{0,n+2} = \boldsymbol{\Phi}(q_{n+2})$, see (28).

Example 2 The one-step error recursion (45) indicates that errors $\mathbf{E}^{\mathbf{r}}_n$ depend strongly on $\mathbf{E}^{\mathbf{r}}_0$ and powers of $\mathbf{T}_+^{-1}\mathbf{T}_0$. This is nicely illustrated by a (pathological) test problem (1) with $k = m = 1$, $G = \mathbb{R}$, $\mathbf{M} \equiv \mathbf{I}$, $\mathbf{g} \equiv \mathbf{0}$ and time dependent constraints $\mathbf{0} = \boldsymbol{\Phi}(q,t) = q - t^3$ that determine the solution completely (no degrees of freedom): If order condition (12) is satisfied, we get $\mathbf{l}^{\mathbf{v}}_n = \mathbf{l}^{\mathbf{a}}_n = \mathbf{0}$ and $\mathbf{l}^q_n = C_q h^3$ with $C_q := 1 - 6\beta - 3(\alpha_m - \alpha_f)$ is constant. Therefore, a straightforward computation shows that the local errors and the higher order error terms in (45) vanish for this test problem and we get $\mathbf{E}^{\mathbf{r}}_n = (\mathbf{T}_+^{-1}\mathbf{T}_0)^n \mathbf{E}^{\mathbf{r}}_0$. Note, that *exact* starting values $\mathbf{v}_0 := \mathbf{v}(t_0) = 3t_0^2$ will result in order reduction (!) since $\mathbf{r}^{\mathbf{B}}_0 = (h\mathbf{e}^{\mathbf{v}}_0 + \mathbf{l}^q_0)/h^2 = C_q h \ne \mathcal{O}(h^2)$, see (35) and (41).

In the general setting of equations of motion (1), the error propagation in the algebraic solution components, see (39) and (45), is coupled to the error propagation in the differential components. Following the approach of Deuflhard et al. [16], we analyse powers of a 2×2 error propagation matrix to get global error bounds for all solution components in DAE time integration.

Lemma 7 *Consider vector valued sequences* $(\mathbf{E}^{\mathbf{y}}_n)_n$, $(\mathbf{E}^{\mathbf{z}}_n)_n$ *that satisfy*

$$\|\mathbf{E}^{\mathbf{y}}_{n+1}\| \le (1 + Lh)\|\mathbf{E}^{\mathbf{y}}_n\| + Lh\|\mathbf{E}^{\mathbf{z}}_n\| + hM, \tag{47a}$$

$$\|\mathbf{E}^{\mathbf{z}}_{n+1} - \mathbf{T}\mathbf{E}^{\mathbf{z}}_n\| \le L\|\mathbf{E}^{\mathbf{y}}_n\| + Lh\|\mathbf{E}^{\mathbf{z}}_n\| + M \tag{47b}$$

with non-negative constants L, M *and a matrix* $\mathbf{T} \in \mathbb{R}^{n_{\mathbf{z}} \times n_{\mathbf{z}}}$ *that has a spectral radius* $\varrho(\mathbf{T}) < 1$.

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There are positive constants C, $\tilde{L}$ and h_0 being independent of n and h such that (47) *implies for all step sizes $h \in (0, h_0]$ the estimates*

$$\|\mathbf{E}_n^{\mathbf{y}}\| \leq C e^{\tilde{L}nh} (\|\mathbf{E}_0^{\mathbf{y}}\| + h\|\mathbf{E}_0^{\mathbf{z}}\| + M), \tag{48a}$$

$$\|\mathbf{E}_n^{\mathbf{z}}\| \leq \|\mathbf{T}^n \mathbf{E}_0^{\mathbf{z}}\| + C e^{\tilde{L}nh} (\|\mathbf{E}_0^{\mathbf{y}}\| + h\|\mathbf{E}_0^{\mathbf{z}}\| + M). \tag{48b}$$

Proof Because of $\varrho(\mathbf{T}) < 1$, there is a norm $\|\mathbf{E}^{\mathbf{z}}\|_\varrho$ in $\mathbb{R}^{n_\mathbf{z}}$ with $\mu := \|\mathbf{T}\|_\varrho < 1$. Norms $\|\mathbf{E}^{\mathbf{z}}\|$ and $\|\mathbf{E}^{\mathbf{z}}\|_\varrho$ are equivalent and we have $\underline{c}\|\mathbf{E}^{\mathbf{z}}\| \leq \|\mathbf{E}^{\mathbf{z}}\|_\varrho \leq \overline{c}\|\mathbf{E}^{\mathbf{z}}\|$, ($\mathbf{E}^{\mathbf{z}} \in \mathbb{R}^{n_\mathbf{z}}$), with suitable positive constants $\underline{c}$, $\overline{c}$.

Using this norm $\|\mathbf{E}^{\mathbf{z}}\|_\varrho$, we define $u_n := \|\mathbf{E}_n^{\mathbf{y}}\|$, $v_n := \|\mathbf{E}_n^{\mathbf{z}} - \mathbf{T}^n\mathbf{E}_0^{\mathbf{z}}\|_\varrho$ and get $v_0 = \|\mathbf{E}_0^{\mathbf{z}} - \mathbf{I}\,\mathbf{E}_0^{\mathbf{z}}\|_\varrho = 0$ and

$$\begin{aligned} v_{n+1} &= \|\mathbf{E}_{n+1}^{\mathbf{z}} - \mathbf{T}\mathbf{E}_n^{\mathbf{z}} + \mathbf{T}(\mathbf{E}_n^{\mathbf{z}} - \mathbf{T}^n\mathbf{E}_0^{\mathbf{z}})\|_\varrho \leq \|\mathbf{E}_{n+1}^{\mathbf{z}} - \mathbf{T}\mathbf{E}_n^{\mathbf{z}}\|_\varrho + \|\mathbf{T}\|_\varrho\, v_n \\ &\leq \overline{c}\|\mathbf{E}_{n+1}^{\mathbf{z}} - \mathbf{T}\mathbf{E}_n^{\mathbf{z}}\| + \mu v_n \leq L_\varrho\|\mathbf{E}_n^{\mathbf{y}}\| + L_\varrho h \cdot \underline{c}\|\mathbf{E}_n^{\mathbf{z}}\| + M_\varrho + \mu v_n \end{aligned}$$

with $L_\varrho := \max\{L, \overline{c}L\}/\min\{1, \underline{c}\}$ and $M_\varrho := \max\{M, \overline{c}M\}$, see (47b). The term $\underline{c}\|\mathbf{E}_n^{\mathbf{z}}\|$ in the right hand side of this estimate is bounded by

$$\underline{c}\|\mathbf{E}_n^{\mathbf{z}}\| \leq \|\mathbf{E}_n^{\mathbf{z}}\|_\varrho \leq v_n + \|\mathbf{T}^n\mathbf{E}_0^{\mathbf{z}}\|_\varrho \leq v_n + \|\mathbf{T}\|_\varrho^n\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho = v_n + \mu^n\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho.$$

Therefore, (47) implies the inequality (to be read componentwise)

$$\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} \leq \begin{pmatrix} 1 + L_\varrho h & L_\varrho h \\ L_\varrho & \mu + L_\varrho h \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} + \begin{pmatrix} \mu^n L_\varrho h\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho + hM_\varrho \\ \mu^n L_\varrho h\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho + M_\varrho \end{pmatrix}. \tag{49}$$

Except the term $\mu^n L_\varrho h\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho$, inequality (49) coincides with related estimates from the literature and may be analysed by similar methods of proof, see [16,21]. Because of $\mu < 1$, the error propagation matrix in (49) has two distinct eigenvalues $\lambda_1 = \mathrm{e}^{\hat{L}h} = 1 + \mathcal{O}(h)$ and $\lambda_2 = \mu + \mathcal{O}(h) < 1$ if the step size $h > 0$ is sufficiently small. Summarizing the corresponding eigenvectors in a transformation matrix $\mathbf{V} = \mathbf{V}(h)$ we get

$$\begin{pmatrix} 1 + L_\varrho h & L_\varrho h \\ L_\varrho & \mu + L_\varrho h \end{pmatrix} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1} \quad \text{with} \quad \mathbf{V} = \begin{pmatrix} \lambda_1 - \mu - L_\varrho h & L_\varrho h \\ L_\varrho & \lambda_2 - 1 - L_\varrho h \end{pmatrix}$$

and $\mathbf{\Lambda} = \mathbf{\Lambda}(h) = \operatorname{diag}(\lambda_1, \lambda_2)$. Because of $\lambda_1^n = \mathrm{e}^{\hat{L}nh}$, $\operatorname{cond}(\mathbf{V}) = \|\mathbf{V}\|\,\|\mathbf{V}^{-1}\| = \mathcal{O}(1)$, $u_0 = \|\mathbf{E}_0^{\mathbf{y}}\|$ and $v_0 = 0$, the iterative application of (49) results in

$$\begin{pmatrix} u_n \\ v_n \end{pmatrix} \leq C_0 \mathrm{e}^{\hat{L}nh}\|\mathbf{E}_0^{\mathbf{y}}\| + \sum_{m=0}^{n-1} \mathbf{V}\mathbf{\Lambda}^m\mathbf{V}^{-1} \begin{pmatrix} \mu^{n-1-m} L_\varrho h\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho + hM_\varrho \\ \mu^{n-1-m} L_\varrho h\|\mathbf{E}_0^{\mathbf{z}}\|_\varrho + M_\varrho \end{pmatrix}$$

with a suitable constant $C_0 > 0$.

To get a bound for $u_n + v_n = \|(u_n, v_n)^\top\|_1$, we consider $\|\mathbf{V}\mathbf{\Lambda}^m\mathbf{V}^{-1}\|_1$, $(m = 0, 1, \ldots, n-1)$, and observe that $\|\mathbf{\Lambda}^m\|_1 = \max\{\lambda_1^m, \lambda_2^m\} \le \mathrm{e}^{\tilde{L}nh}$ with $\tilde{L} := |\hat{L}|$. Therefore, $\|\mathbf{V}\mathbf{\Lambda}^m\mathbf{V}^{-1}\|_1$ is uniformly bounded and

$$\sum_{m=0}^{n-1} \|\mathbf{V}\mathbf{\Lambda}^m\mathbf{V}^{-1}\|_1 \cdot \mu^{n-1-m} L_\varrho h \|\mathbf{E}_0^\mathbf{z}\|_\varrho \le \hat{C}\mathrm{e}^{\tilde{L}nh} \cdot h\|\mathbf{E}_0^\mathbf{z}\|$$

with $\hat{C} := \bar{c}L_\varrho \operatorname{cond}_1(\mathbf{V})/(1-\mu)$ follows from $\mu < 1$ and $\|\mathbf{E}_0^\mathbf{z}\|_\varrho \le \bar{c}\|\mathbf{E}_0^\mathbf{z}\|$. Estimating finally the error terms that arise from hM_ϱ and M_ϱ in the same way as in Lemma VI.3.9 of [21], we get

$$\|\mathbf{E}_n^\mathbf{y}\| + \|\mathbf{E}_n^\mathbf{z} - \mathbf{T}^n\mathbf{E}_0^\mathbf{z}\|_\varrho = u_n + v_n \le \tilde{C}\mathrm{e}^{\tilde{L}nh}(\|\mathbf{E}_0^\mathbf{y}\| + h\|\mathbf{E}_0^\mathbf{z}\| + M_\varrho)$$

with a suitable constant $\tilde{C} > 0$. Because of $\|\mathbf{E}_n^\mathbf{z} - \mathbf{T}^n\mathbf{E}_0^\mathbf{z}\| \le \|\mathbf{E}_n^\mathbf{z} - \mathbf{T}^n\mathbf{E}_0^\mathbf{z}\|_\varrho/\underline{c}$ and $M_\varrho \le M/\max\{1, \bar{c}\}$, the estimates (48) follow straightforwardly. □

The contractivity condition $\varrho(\mathbf{T}) < 1$ is one of the crucial assumptions of Lemma 7. In the convergence analysis of Theorems 1 and 2, it has to be verified for two different matrices $\mathbf{T}$. Parameters $\alpha_m, \alpha_f, \beta, \gamma$ have to satisfy stability conditions to guarantee $\varrho(\mathbf{T}) < 1$ in both convergence theorems:

Lemma 8 (a) *The order condition* (12) *and the stability conditions*

$$\alpha_m < \alpha_f < \frac{1}{2}, \quad \beta > \frac{1}{4} + \frac{1}{2}(\alpha_f - \alpha_m) \tag{50}$$

guarantee that $\beta \ne 0$, $\gamma > 1/2$ *and the contractivity conditions*

$$\left|\frac{\alpha_m}{1-\alpha_m}\right| < 1, \quad \left|\frac{\alpha_f}{1-\alpha_f}\right| < 1, \quad \left|\frac{1-\gamma}{\gamma}\right| < 1, \quad \varrho(\mathbf{T}_+^{-1}\mathbf{T}_0) < 1 \tag{51}$$

are satisfied.

(b) *For the "optimal" parameters of Chung and Hulbert* [14]

$$\alpha_m = \frac{2\rho_\infty - 1}{\rho_\infty + 1}, \quad \alpha_f = \frac{\rho_\infty}{\rho_\infty + 1}, \quad \gamma = \frac{1}{2} + \alpha_f - \alpha_m, \quad \beta = \frac{1}{4}\left(\gamma + \frac{1}{2}\right)^2 \tag{52}$$

the stability conditions (50) *are satisfied for any* $\rho_\infty \in [0, 1)$.

Proof Lemma 1 of [3] analyses the stability of generalized-α methods at infinity. Conditions (12) and (50) are used to prove that all roots ζ_i of polynomial $\sigma(\zeta) := \det(\zeta\mathbf{T}_+ - \mathbf{T}_0)$ are inside the unit circle. Since (50) implies that $\mathbf{T}_+$ is non-singular, matrix $\mathbf{T}_+^{-1}\mathbf{T}_0$ is well defined. Its characteristic polynomial is $\det(\mathbf{T}_+^{-1}\mathbf{T}_0 - \zeta\mathbf{I}) = -\det(\mathbf{T}_+^{-1})\sigma(\zeta)$ and we get $\varrho(\mathbf{T}_+^{-1}\mathbf{T}_0) = \max_i |\zeta_i| < 1$. The remaining contractivity conditions follow from $\alpha_m < 1/2$ and $\gamma > 1/2$, respectively. The proof of (b) is given in [3, Section 2]. □

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Theorem 1 *Let the order condition* (12) *and the stability conditions* (50) *be fulfilled and suppose* $\theta = \max\{\|\mathbf{\Phi}(q_m)\| \,:\, m \geq 0,\ t_0 + mh \leq t_{\text{end}}\} = \mathcal{O}(h^{3+\varepsilon})$ *for some* $\varepsilon > 0$. *If the starting values* q_0, $\mathbf{v}_0$, $\dot{\mathbf{v}}_0$, $\mathbf{a}_0$ *and* $\boldsymbol{\lambda}_0$ *satisfy*

$$\|\mathbf{M}(q_0)\dot{\mathbf{v}}_0 + \mathbf{g}(q_0, \mathbf{v}_0, t_0) + \mathbf{B}^\top(q_0)\boldsymbol{\lambda}_0\| = \mathcal{O}(h^{1+\delta}), \quad \|\mathbf{e}_0^{\mathbf{v}}\| = \mathcal{O}(h^2),$$
$$\|\mathbf{e}_0^q\| + \|\mathbf{e}_0^{\mathbf{Bv}} + \frac{1}{h}\mathbf{B}(q(t_0))\mathbf{l}_0^q\| + h\|\mathbf{e}_0^{\dot{\mathbf{v}}}\| + h\|\mathbf{e}_0^{\mathbf{a}}\| = \mathcal{O}(h^{2+\delta}) \tag{53}$$

with a non-negative constant $\delta \in [0, 1]$ *and* $\theta = \mathcal{O}(h^{3+\max(\delta,\varepsilon)})$, *then the global errors are bounded by*

$$\|\mathbf{e}_n^q\| + \|\mathbf{e}_n^{\mathbf{v}}\| \leq C_0 e^{\tilde{L}(t_n - t_0)}(\theta/h^2 + h^2), \tag{54a}$$
$$\|\mathbf{e}_n^{\boldsymbol{\lambda}}\| + \|\mathbf{e}_n^{\dot{\mathbf{v}}}\| + \|\mathbf{e}_n^{\mathbf{a}}\| \leq C_0 \left(\|\mathbf{T}^n\| h^{1+\delta} + e^{\tilde{L}(t_n - t_0)}(\theta/h^2 + h^2)\right) \tag{54b}$$

if $h \in (0, h_0]$ *and* $t_0 + nh \leq t_{\text{end}} - h$. *Here, the positive constants* C_0, $\tilde{L}$ *and* h_0 *are independent of* n *and* h *and* $\mathbf{T} :=$ *blockdiag* $(-\alpha_m/(1-\alpha_m),\ \mathbf{T}_+^{-1}\mathbf{T}_0)$.

Proof We study the coupled propagation of errors $\mathbf{E}_n^{\mathbf{y}} := ((\mathbf{e}_n^q)^\top,\ (\mathbf{e}_n^{\mathbf{v}})^\top)^\top$ in differential solution components and errors $\mathbf{E}_n^{\mathbf{z}} := ((\mathbf{e}_n^{\mathbf{Pa}})^\top,\ (\mathbf{E}_n^{\mathbf{r}})^\top)^\top$ in algebraic solution components, see Lemma 7.

Taking into account that $\varepsilon_n = \mathcal{O}(1)(\|\mathbf{E}_n^{\mathbf{y}}\| + h\|\mathbf{E}_n^{\mathbf{z}}\|)$, Lemma 2 yields

$$\mathbf{E}_{n+1}^{\mathbf{y}} = \mathbf{E}_n^{\mathbf{y}} + \mathcal{O}(h)(\|\mathbf{E}_n^{\mathbf{y}}\| + \|\mathbf{E}_n^{\mathbf{z}}\| + \|\mathbf{E}_{n+1}^{\mathbf{z}}\|) + \mathcal{O}(h^3). \tag{55a}$$

Next, we multiply (39) and (45) by $1/(1-\alpha_m)$ and $\|(\mathbf{T}_+^{-1} \otimes \mathbf{I}_m)\|$, respectively, and get

$$\begin{aligned}\|\mathbf{e}_{n+1}^{\mathbf{Pa}} - \frac{\alpha_m}{1-\alpha_m}\mathbf{e}_n^{\mathbf{Pa}}\| + \|\mathbf{E}_{n+1}^{\mathbf{r}} - (\mathbf{T}_+^{-1}\mathbf{T}_0 \otimes \mathbf{I}_m)\mathbf{E}_n^{\mathbf{r}}\| \\ \leq \mathcal{O}(1)(\|\mathbf{E}_n^{\mathbf{y}}\| + \|\mathbf{E}_{n+1}^{\mathbf{y}}\| + h\|\mathbf{E}_n^{\mathbf{z}}\| + h\|\mathbf{E}_{n+1}^{\mathbf{z}}\|) + \mathcal{O}(h^{-2})\theta + \mathcal{O}(h^2).\end{aligned} \tag{55b}$$

From (55a), (55b) and the definition of $\mathbf{T}$ above, estimates (47a) and (47b) are obtained by setting $M := M_0(\theta/h^2 + h^2)$ with some constant $M_0 > 0$. Conditions (53) result in $\|\mathbf{E}_0^{\mathbf{y}}\| = \mathcal{O}(h^2)$, $\|\mathbf{E}_0^{\mathbf{z}}\| = \mathcal{O}(h^{1+\delta})$ since $\|\mathbf{e}_0^{\mathbf{a}}\| = \mathcal{O}(h^{1+\delta})$, $\|\mathbf{e}_0^{\mathbf{S}\boldsymbol{\lambda}}\| = \|\mathbf{e}_0^{\dot{\mathbf{v}}}\| + \mathcal{O}(h^2) = \mathcal{O}(h^{1+\delta})$ and

$$\|\mathbf{r}_0^{\mathbf{B}}\| = \mathcal{O}(1)\left((\|\mathbf{e}_0^q\| + \|\mathbf{e}_0^{\mathbf{Bv}} + \mathbf{B}(q(t_0))\mathbf{l}_0^q/h\|)/h + \varepsilon_0 + \theta/h^2\right) + \mathcal{O}(h^2),$$

i.e., $\|\mathbf{r}_0^{\mathbf{B}}\| = \mathcal{O}(1)\theta/h^2 + \mathcal{O}(h^{1+\delta}) = \mathcal{O}(h^{1+\delta})$, see (35), (41) and (53). The contractivity conditions (Lemma 8) yield $\varrho(\mathbf{T}) < 1$.

Error bound (48a) proves assertion (54a) since $\|\mathbf{e}_n^q\| + \|\mathbf{e}_n^{\mathbf{v}}\| = \mathcal{O}(1)\|\mathbf{E}_n^{\mathbf{y}}\|$. The corresponding result for the algebraic components is obtained from (48b) since $\|\mathbf{e}_n^{\boldsymbol{\lambda}}\|$, $\|\mathbf{e}_n^{\dot{\mathbf{v}}}\|$, $\|\mathbf{e}_n^{\mathbf{a}}\|$ are bounded by $\mathcal{O}(1)\|\mathbf{E}_n^{\mathbf{z}}\|$, see (44) and Lemma 3. □

Remark 3 (a) For the trivial choice $\mathbf{v}_0 := \mathbf{v}(t_0)$, the assumptions of Theorem 1 are satisfied only with $\delta = 0$ if $\|\mathbf{B}(q(t_0))\mathbf{l}_0^q\| = \mathcal{O}(h^3)$. The resulting first order error term $C_0\|\mathbf{T}^n\|h$ in (54b) indicates the risk of order reduction. This is in very good agreement with the numerical test results in Example 1 since $\|\mathbf{B}(q(t_0))\mathbf{l}_0^q\| = \mathcal{O}(h^3)\|[\mathbf{B}(q)\ddot{\mathbf{v}}](t_0)\| + \mathcal{O}(h^4)$ in linear spaces, see (17). For the mathematical pendulum, the leading error term is $[\mathbf{B}(q)\ddot{\mathbf{v}}](t_0) = -3gx_0\dot{x}_0/y_0$. It vanishes in the equilibrium position $x_0 = 0$ resulting in $\delta = 1$ (no order reduction) but introduces a first order error term in the transient phase if $x_0 = 0.2$ (order reduction), see Fig. 1.

(b) The block structure of $\mathbf{E}_n^{\mathbf{z}}$ and the 2×2 block diagonal structure of matrix $\mathbf{T}$ in Theorem 1 allow to relax the assumptions on $\mathbf{e}_0^{\mathbf{a}}$. If $\|\mathbf{e}_0^{\mathbf{Ba}}\| = \mathcal{O}(h^{1+\delta})$ and $\|\mathbf{e}_0^{\mathbf{Pa}}\| = \mathcal{O}(h^{1+\delta_{\mathbf{P}}})$ with $0 \le \delta_{\mathbf{P}} \le \delta$ then estimate (54b) remains valid for error components $\mathbf{e}_n^{\boldsymbol{\lambda}}$, $\mathbf{e}_n^{\dot{\mathbf{v}}}$, and $\mathbf{e}_n^{\mathbf{Ba}}$. For error component $\mathbf{e}_n^{\mathbf{Pa}}$, we get a similar error bound with δ being replaced by $\delta_{\mathbf{P}}$. For the mathematical pendulum in equilibrium position $x_0 = 0$, we have $[\mathbf{B}(q)\ddot{\mathbf{v}}](t_0) = 0$ and the trivial choice $\mathbf{a}_0 := \dot{\mathbf{v}}(t_0)$ does not affect the second order convergence in components q, $\mathbf{v}$ and $\boldsymbol{\lambda}$ since $\delta_{\mathbf{P}} = 0$ but $\|\mathbf{e}_0^{\mathbf{Ba}}\| = \mathcal{O}(h^2)$, i.e., $\delta = 1$.

4 Improved transient behaviour and stabilization by index reduction

Based on Theorem 1, we study in the present section the large transient errors of the generalized-α method (9) and show how to avoid them by carefully selected starting values $\mathbf{v}_0$, $\mathbf{a}_0$ or by index reduction.

4.1 Spurious oscillations in the transient phase: analysis

The global error bounds (54) are composed of three parts: The well known second order convergence result [3,10] is reflected by the term $e^{\tilde{L}(t_n-t_0)}h^2$. The term $e^{\tilde{L}(t_n-t_0)}\theta/h^2$ with $\theta = \max_m \|\boldsymbol{\Phi}(q_m)\|$ illustrates the amplification of (small) residuals in algebraic constraints that is typical of ODE methods being directly applied to the index-3 formulation of the equations of motion (1), see [1]. Finally, the large errors in the transient phase, see Example 1, correspond to the error term $\|\mathbf{T}^n\|h^{1+\delta}$ in (54b) that is dominated by $\|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\|h^{1+\delta}$ since $\mathbf{T} = \text{blockdiag}\,(-\alpha_m/(1-\alpha_m),\ \mathbf{T}_+^{-1}\mathbf{T}_0)$ and $(-\alpha_m/(1-\alpha_m))^n$ decays rapidly, see (51).

Condition $\varrho(\mathbf{T}_+^{-1}\mathbf{T}_0) < 1$ in Lemma 8 implies $\lim_{n\to\infty}(\mathbf{T}_+^{-1}\mathbf{T}_0)^n = \mathbf{0}$ but for non-normal matrices $\mathbf{T}_+^{-1}\mathbf{T}_0$ it is well known that $\max_n \|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\|$ and the terms $\|\mathbf{T}^n\mathbf{E}_0^{\mathbf{z}}\|$, $\|\mathbf{T}^n\|$ in error bounds (48b) and (54b) may nevertheless become very large. In 1978, Hilber and Hughes [22] characterized a similar phenomenon as "overshooting" of Newmark type methods in the application to the unconstrained scalar test equation $\ddot{q} + \omega^2 q = 0$. In that case, $\dot{v}_n = -\omega^2 q_n$ and a straightforward analysis shows that the numerical solution follows a recursion $\mathbf{T}_+(z)\mathbf{E}_{n+1} = \mathbf{T}_0(z)\mathbf{E}_n$ with $\mathbf{E}_n = (hv_n, z^2q_n, h^2a_n)^\top$, $z := h\omega$ and $\lim_{z\to\infty}\mathbf{T}_+(z) = \mathbf{T}_+$, $\lim_{z\to\infty}\mathbf{T}_0(z) = \mathbf{T}_0$. For parameters $\alpha_m, \alpha_f, \beta, \gamma$ according to (52) with $\rho_\infty \in [0, 1)$, the stability estimate $\varrho((\mathbf{T}_+(z))^{-1}\mathbf{T}_0(z)) < 1$, $(z > 0)$, proves $\lim_{n\to\infty}\mathbf{E}_n = \mathbf{0}$ for any starting vector

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$\mathbf{E}_0 = (hv_0, z^2 q_0, h^2 a_0)^\top$, see [14]. However, in a transient phase $\|\mathbf{E}_n\|$ may become much larger than $\|\mathbf{E}_0\|$ if the initial displacements q_0 do not vanish [22].

For the application of Newmark type methods to constrained systems an error amplification by powers of the non-normal matrix $\mathbf{T}_+^{-1}\mathbf{T}_0$ has already been observed in 1994, see [12]. For the more detailed convergence analysis of the present paper we have to study terms $((\mathbf{T}_+^{-1}\mathbf{T}_0)^n \otimes \mathbf{I}_m)\mathbf{E}_0^{\mathbf{r}} \in \mathbb{R}^{3m}$ that are composed of (scaled) global errors in velocity and acceleration coordinates and in Lagrange multipliers, see (44). For exact starting values $q_0 := q(t_0)$, $\mathbf{v}_0 := \mathbf{v}(t_0)$, $\dot{\mathbf{v}}_0 := \dot{\mathbf{v}}(t_0)$, $\boldsymbol{\lambda}_0 := \boldsymbol{\lambda}(t_0)$ and $\mathbf{a}_0 := \dot{\mathbf{v}}(t_0 + \Delta_\alpha h)$, this sequence is initialized by $\mathbf{E}_0^{\mathbf{r}} = ((\mathbf{r}_0^{\mathbf{B}})^\top, \mathbf{0}, \mathbf{0})^\top$ with $\mathbf{r}_0^{\mathbf{B}} = \mathbf{B}(q(t_0))\mathbf{l}_0^q / h^2 + \mathcal{O}(h^2)$ and results in general in a first order error term $C_0\|\mathbf{T}^n\|h$ for components $\boldsymbol{\lambda}$ that disappears only if $\mathbf{B}(q(t_0))\mathbf{l}_0^q = \mathcal{O}(h^4)$, see (54b) and Remark 3 above.

In practical applications, parameters $\alpha_m, \alpha_f, \beta, \gamma$ according to (52) are very popular since they allow to adjust the "numerical damping properties" for linear problems $\ddot{q} + \omega^2 q = 0$ by just one single parameter ρ_∞, see [14]. With (52), the error amplification matrix $\mathbf{T}_+^{-1}\mathbf{T}_0 \in \mathbb{R}^{3\times 3}$ has an eigenvalue $\mu = -\rho_\infty$ of multiplicity three. The Jordan canonical form is given by $\mathbf{T}_+^{-1}\mathbf{T}_0 = \mathbf{X}\mathbf{J}\mathbf{X}^{-1}$ with

$$\mathbf{J} := \begin{pmatrix} \mu & 1 & 0 \\ 0 & \mu & 1 \\ 0 & 0 & \mu \end{pmatrix}, \quad \mathbf{X} := \begin{pmatrix} 0 & \frac{1}{2}\frac{1+\mu}{1-\mu} & -\frac{1}{(1-\mu)^2} \\ 1-\mu^2 & -(2+\mu) & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

resulting in $(\mathbf{T}_+^{-1}\mathbf{T}_0)^n = \mathbf{X}\mathbf{J}^n\mathbf{X}^{-1}$ and $\|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\| \geq \|\mathbf{J}^n\|/\mathrm{cond}\,(\mathbf{X})$. It may be verified by induction that the non-zero elements of $\mathbf{J}^n$, $(n \geq 2)$, are given by μ^n, $n\mu^{n-1}$ and $n(n-1)\mu^{n-2}/2$. Consequently, $\max_n \|\mathbf{J}^n\|_\infty$ is bounded from below by $c_\infty := \max_n n(n-1)\rho_\infty^{n-2}/2$. Typical values are $c_\infty = 2.2$, $c_\infty = 28.5$ and $c_\infty = 2.7 \times 10^3$ for $\rho_\infty = 0.6$, $\rho_\infty = 0.9$ and $\rho_\infty = 0.99$, respectively.

Because $\|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\|$ may become very large, the global error bound (54b) is dominated in the transient phase by $\|\mathbf{T}^n\|h^{1+\delta}$. (This term does not contribute significantly to the global error in long-term integration since $\varrho(\mathbf{T}) < 1$, see [3,10].) For the numerical test in Example 1, we have $\rho_\infty = 0.9$ and the norm $\|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\|_2$ reaches its maximum value 34.3 at $n = 14$ which is in very good agreement with $\max_n \|\mathbf{e}_n^{\boldsymbol{\lambda}}\| = \|\mathbf{e}_{15}^{\boldsymbol{\lambda}}\|$, see Fig. 1. In the parameter range of interest ($\rho_\infty \in [0.3, 0.99]$), the maximum amplification factor may be approximated with a relative error $< 3\%$ by $\max_n \|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\|_2 \approx 0.9/(1 - \rho_\infty^{0.25})$ illustrating the risk of significant spurious oscillations in the transient phase for generalized-α methods with small amount of numerical damping since $1 - \rho_\infty^{0.25} \ll 1$ in that case.

4.2 Perturbing the starting values to improve the transient behaviour

The default initialization $q_0 = q(t_0)$, $\mathbf{v}_0 = \mathbf{v}(t_0)$ in (9) may result in large transient errors in $\boldsymbol{\lambda}$ because of order reduction. The refined local error analysis of generalized-α methods [25], see also Lemma 1 above, shows that starting values $\mathbf{a}_0 = \dot{\mathbf{v}}(t_0 + \Delta_\alpha h) + \mathcal{O}(h^2)$ are more favourable than the brute force approach $\mathbf{a}_0 = \dot{\mathbf{v}}(t_0)$ in [17]. Guided

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by Theorem 1, we propose in the present section an additional perturbation of size $\mathcal{O}(h^2)$ for starting values $\mathbf{v}_0$ to avoid order reduction in the direct application of the Lie group integrator (9) to the index-3 formulation (1) of the equations of motion.

In Theorem 1, the assumptions (53) on $\mathbf{e}_0^{\mathbf{v}}$ may be satisfied with $\delta = 1$ (no order reduction) setting

$$\mathbf{v}_0 := \mathbf{v}(t_0) + \boldsymbol{\Delta}_0^{\mathbf{v}} \quad \text{with} \quad \boldsymbol{\Delta}_0^{\mathbf{v}} = \mathbf{M}_0^{-1}\mathbf{B}_0^\top(\mathbf{B}_0\mathbf{M}_0^{-1}\mathbf{B}_0^\top)^{-1}\mathbf{B}_0\mathbf{l}_0^q/h + \mathcal{O}(h^3). \tag{56}$$

Because of $\|\mathbf{e}_0^q\| = \mathcal{O}(h^{2+\delta})$, it is not relevant if matrices $\mathbf{B}_0, \mathbf{M}_0$ in (56) are evaluated at $q = q(t_0)$ or at $q = q_0$. For given $\mathbf{B}_0\mathbf{l}_0^q/h \in \mathbb{R}^m$, the update vector $\boldsymbol{\Delta}_0^{\mathbf{v}} \in \mathbb{R}^k$ in (56) may be computed solving a linear 2×2 block system of type (7) since $\mathbf{M}_0\boldsymbol{\Delta}_0^{\mathbf{v}} + \mathbf{B}_0^\top\boldsymbol{\Delta}_0^{\boldsymbol{\lambda}} = \mathbf{0}$ and $\mathbf{B}_0\boldsymbol{\Delta}_0^{\mathbf{v}} = \mathbf{B}_0\mathbf{l}_0^q/h$ with the auxiliary vector $\boldsymbol{\Delta}_0^{\boldsymbol{\lambda}} = -(\mathbf{B}_0\mathbf{M}_0^{-1}\mathbf{B}_0^\top)^{-1}\mathbf{B}_0\mathbf{l}_0^q/h \in \mathbb{R}^m$. I.e., substituting $-\mathbf{g}_0 \to \mathbf{0}$, $-\mathbf{R}_0 \to \mathbf{B}_0\mathbf{l}_0^q/h$ in (7), we get instead of $\dot{\mathbf{v}}(t_0)$, $\boldsymbol{\lambda}(t_0)$ the update vector $\boldsymbol{\Delta}_0^{\mathbf{v}}$ (and $\boldsymbol{\Delta}_0^{\boldsymbol{\lambda}}$ that is not needed in the following).

To get an approximation of $\mathbf{l}_0^q$, we consider the leading error term in (17) that is composed of $[\widetilde{\mathbf{v}}(t_0), \widetilde{\dot{\mathbf{v}}}(t_0)]$ and a multiple of $\widetilde{\ddot{\mathbf{v}}}(t_0)$. The commutator is evaluated for the known initial values $\mathbf{v}(t_0)$, $\dot{\mathbf{v}}(t_0)$, see (7). The term $\ddot{\mathbf{v}}(t_0)$ may be approximated by finite differences using vectors $\dot{\mathbf{v}}_{\pm sh} \approx \dot{\mathbf{v}}(t_0 \pm sh)$ with some $s \in (0, 1]$ that are obtained from (7) substituting the arguments $q(t_0)$, $\mathbf{v}(t_0)$, t_0 of $\mathbf{M}_0$, $\mathbf{B}_0$, $\mathbf{g}_0$, $\mathbf{R}_0$ by $q_{\pm sh} := q(t_0) \circ \exp(\pm sh\mathbf{v}(t_0) + s^2h^2\dot{\mathbf{v}}(t_0)/2)$, $\mathbf{v}_{\pm sh} := \mathbf{v}(t_0) \pm sh\dot{\mathbf{v}}(t_0)$ and $t_0 \pm sh$, respectively.

Second order differences $(\dot{\mathbf{v}}_{sh} - \dot{\mathbf{v}}_{-sh})/(2sh)$ require two function evaluations of $\mathbf{M}$, $\mathbf{B}$, $\mathbf{g}$, $\mathbf{R}$ and the solution of two linear systems (7) but are more accurate than first order differences $(\dot{\mathbf{v}}_{sh} - \dot{\mathbf{v}}(t_0))/(sh)$ that need 50% less numerical effort. The additional numerical effort arises, however, only once to define appropriate starting values $\mathbf{v}_0$, $\mathbf{a}_0$. In the numerical tests, parameters $s = 1$ (second order differences) and $s = 0.01$ (first order differences) were found to be appropriate. The finite difference approximation of $\ddot{\mathbf{v}}(t_0)$ is used as well to define starting values

$$\mathbf{a}_0 := \dot{\mathbf{v}}(t_0) + \Delta_\alpha h\ddot{\mathbf{v}}(t_0) = \dot{\mathbf{v}}(t_0 + \Delta_\alpha h) + \mathcal{O}(h^2) \tag{57}$$

that satisfy assumption (53) in Theorem 1 with the optimal value $\delta = 1$.

For the mathematical pendulum with $x_0 = 0.2$ (Example 1), the maximum global errors $\|\mathbf{e}_n^{\boldsymbol{\lambda}}\|$ in $t \in [0, 2]$ are reduced from 2.48×10^{-1} to 3.99×10^{-3} (for $h = 2.0 \times 10^{-2}$) and from 1.23×10^{-1} to 9.96×10^{-4} (for $h = 10^{-2}$) if the generalized-α method (9) is initialized with perturbed starting values $\mathbf{v}_0$, $\mathbf{a}_0$ according to (56), (57). For $x_0 = 0$ and $t_n \in [0, 2]$ we observe $\|\mathbf{e}_n^{\boldsymbol{\lambda}}\| \le 3.95 \times 10^{-3}$ for step size $h = 2.0 \times 10^{-2}$ and $\|\mathbf{e}_n^{\boldsymbol{\lambda}}\| \le 9.85 \times 10^{-4}$ for step size $h = 10^{-2}$, both for starting values $\mathbf{v}_0 = \mathbf{v}(t_0)$, $\mathbf{a}_0 = \dot{\mathbf{v}}(t_0)$ and for starting values $\mathbf{v}_0$, $\mathbf{a}_0$ according to (56), (57), see the detailed discussion in Remark 3.

It is an interesting detail that the well known improved starting values $\mathbf{a}_0$ according to (57), see [25], do not fix the order reduction problem in the direct application of (9) to the index-3 formulation (1). For small numerical damping ($\rho_\infty \ge 0.9$), the benefits of perturbed starting values $\mathbf{v}_0$ are larger by a factor > 100 than the influence of $\mathbf{e}_0^{\mathbf{a}}$. This is justified by the observation that $\mathbf{E}_n^{\mathbf{r}} \approx (\mathbf{T}_+^{-1}\mathbf{T}_0)^n\mathbf{E}_0^{\mathbf{r}}$ in the transient

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phase, see (48b). For $\mathbf{e}_n^{\boldsymbol{\lambda}}$, we have to consider the maximum entries of the second row of $(\mathbf{T}_+^{-1}\mathbf{T}_0)^n$, see (44). For $\rho_\infty = 0.9$, these are given by $(31.91,\ 0.81,\ 0.31)$ with $31.91/0.31 > 100$.

4.3 Stabilized index-2 formulation

Notation (9) suggests a straightforward generalization of the Gear–Gupta–Leimkuhler formulation [18] (also known as stabilized index-2 formulation [5]) to the Lie group setting [4]: The introduction of auxiliary variables $\boldsymbol{\eta}_n \in \mathbb{R}^m$ in the update $\boldsymbol{\Delta}\mathbf{q}_n$ for the position coordinates q_n allows to enforce additionally at $t = t_{n+1}$ the hidden constraints (3) at the level of velocity coordinates. For this purpose, the update $\boldsymbol{\Delta}\mathbf{q}_n$ in (9b) is substituted by

$$\boldsymbol{\Delta}\mathbf{q}_n = \mathbf{v}_n - \mathbf{B}^\top(q_n)\boldsymbol{\eta}_n + (0.5-\beta)h\mathbf{a}_n + \beta h\mathbf{a}_{n+1}, \tag{58a}$$

$$\mathbf{B}(q_{n+1})\mathbf{v}_{n+1} = \mathbf{0}. \tag{58b}$$

Theorem 2 *For the stabilized index-2 formulation, the assertions of Theorem 1 remain valid with* θ/h^2 *being substituted by* $\bar\theta/h$ *with* $\bar\theta := \max_m \|\boldsymbol{\Phi}(q_m)\| + \max_m \|\mathbf{B}(q_m)\mathbf{v}_m\| = \mathcal{O}(h^{2+\varepsilon})$ *and* $\bar\theta = \mathcal{O}(h^{2+\max(\delta,\varepsilon)})$ *if the assumptions on the starting values* q_0, $\mathbf{v}_0$ *are relaxed to* $\|\mathbf{e}_0^q\| + \|\mathbf{e}_0^{\mathbf{v}}\| = \mathcal{O}(h^2)$ *and matrix* $\mathbf{T}$ *in (54b) is defined by* $\mathbf{T} \in \mathbb{R}^{3\times 3}$ *with* $\mathbf{T} := \mathrm{blockdiag}\,(-\alpha_m/(1-\alpha_m),\ \mathbf{T}_+^{-1}\mathbf{T}_0)$ *and*

$$\mathbf{T}_+ = \begin{pmatrix} 0 & -\gamma \\ 1-\alpha_f & 1-\alpha_m \end{pmatrix}, \quad \mathbf{T}_0 = \begin{pmatrix} 0 & 1-\gamma \\ -\alpha_f & -\alpha_m \end{pmatrix}. \tag{59}$$

Proof The convergence analysis follows step by step the analysis for the Lie group method (9) in the original index-3 formulation of the equations of motion. In the definition of local errors, see (10), a term $-\mathbf{B}^\top(q(t_n))\boldsymbol{\eta}(t_n)$ with $\boldsymbol{\eta}(t) \equiv \mathbf{0}$ is formally added to the right hand side of (10b). Then, a new error term $-\widetilde{\mathbf{e}}_n^{\mathbf{B}^\top\boldsymbol{\eta}} + \mathcal{O}(h)\|\widetilde{\mathbf{e}}_n^{\boldsymbol{\eta}}\|$ appears in the right hand side of estimate (23). Multiplying (23) by $\mathbf{B}(q(t_n))$, we get

$$-\,\mathbf{e}_n^{\mathbf{B}\mathbf{B}^\top\boldsymbol{\eta}} = \mathbf{B}\,(q(t_n))\,\boldsymbol{\Delta}_h\mathbf{e}_n^q + \mathcal{O}(1)(\varepsilon_n + h\|\mathbf{e}_n^{\boldsymbol{\eta}}\| + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|) + \mathcal{O}(h^2). \tag{60}$$

The time discrete approximation (27) of the hidden constraints at the level of acceleration coordinates allows to substitute in (60) the term $\mathbf{B}(q(t_n))\boldsymbol{\Delta}_h\mathbf{e}_n^q$ by $\mathcal{O}(1)(\varepsilon_n + h\|\boldsymbol{\Delta}_h\mathbf{e}_n^q\| + \|\mathbf{D}_{1,n}\|)$ resulting in an error bound

$$\|\mathbf{e}_n^{\boldsymbol{\eta}}\| = \mathcal{O}(1)(\varepsilon_n + h\|\boldsymbol{\Delta}_h\mathbf{e}_n^q\| + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\| + \|\mathbf{D}_{1,n}\|) + \mathcal{O}(h^2) \tag{61}$$

since $[\mathbf{B}\mathbf{B}^\top](q) \in \mathbb{R}^{m\times m}$ is non-singular for any full rank matrix $\mathbf{B}(q)$. Therefore, $\mathbf{e}_n^{\boldsymbol{\eta}}$ contributes in (20) only to higher order error terms and to the local error that gets the form $\mathcal{O}(h)\|\mathbf{D}_{1,n}\| + \mathcal{O}(h^3) = \mathcal{O}(h)(\bar\theta/h + h^2)$. In (23), error term $-\widetilde{\mathbf{e}}_n^{\mathbf{B}^\top\boldsymbol{\eta}}$ may be considered substituting $\widetilde{\mathbf{l}}_n^q/h$ by $\widetilde{\mathbf{l}}_n^q/h + \mathcal{O}(1)(\bar\theta/h + h^2)$.

Because of the hidden constraints (3), we have $\mathbf{B}(q(t_n))\mathbf{v}(t_n) = \mathbf{0}$ and get with the notations of the proof of Lemma 4

$$-\mathbf{B}(q_n)\mathbf{v}_n = \mathbf{B}(q_n)\mathbf{e}_n^{\mathbf{v}} - \big(\mathbf{B}(q_{n,1}) - \mathbf{B}(q_{n,0})\big)\,\mathbf{v}(t_n)$$

$$= \mathbf{e}_n^{\mathbf{Bv}} + \mathcal{O}(h)\|\mathbf{e}_n^{\mathbf{v}}\| + \int_0^1 \mathbf{R}(q_{n,\vartheta})\,\big(\mathbf{v}(t_n), \mathbf{e}_n^{q}\big)\,\mathrm{d}\vartheta.$$

Therefore, the difference $\mathbf{e}_{n+1}^{\mathbf{Bv}} - \mathbf{e}_n^{\mathbf{Bv}}$ is bounded in terms of $\|\mathbf{B}(q_{n+1})\mathbf{v}_{n+1}\|$, $\|\mathbf{B}(q_n)\mathbf{v}_n\|$, $h\|\mathbf{e}_{n+1}^{\mathbf{v}}\|$, $h\|\mathbf{e}_n^{\mathbf{v}}\|$, $h\|\mathbf{\Delta}_h\mathbf{e}_n^{q}\|$ and $h\|\mathbf{e}_n^{q}\|$. Multiplying (21) by matrix $\mathbf{B}(q(t_n))$ and scaling this expression by $1/h$, we obtain

$$(1-\gamma)\mathbf{e}_n^{\mathbf{Ba}} + \gamma\mathbf{e}_{n+1}^{\mathbf{Ba}} = \frac{\mathbf{e}_{n+1}^{\mathbf{Bv}} - \mathbf{e}_n^{\mathbf{Bv}}}{h} + \mathcal{O}(1)(\|\mathbf{e}_{n+1}^{\mathbf{v}}\| + h\|\mathbf{e}_{n+1}^{\mathbf{a}}\|) + \mathcal{O}(h^2),$$

$$= \mathcal{O}(1)\bar{\theta}/h + \mathcal{O}(1)(\varepsilon_n + \varepsilon_{n+1}) + \mathcal{O}(h^2).$$

This one-step recursion for errors $\mathbf{e}_n^{\mathbf{Ba}}$ substitutes (42) and there is no need to consider vectors $\mathbf{r}_n^{\mathbf{B}}$ in the convergence analysis for the stabilized index-2 formulation. With the modified definition $\mathbf{E}_n^{\mathbf{r}} := ((\mathbf{e}_n^{\mathbf{S\lambda}})^\top, (\mathbf{e}_n^{\mathbf{Ba}})^\top)^\top$, see (44), the remaining part of the convergence analysis follows line by line the analysis of Sect. 3. □

Remark 4 (a) The error bound $\|\boldsymbol{\eta}_n\| = \|\mathbf{e}_n^{\boldsymbol{\eta}}\| = \mathcal{O}(1)\bar{\theta}/h + \mathcal{O}(h^2)$ is a straightforward consequence of (61), see also [4]. In that paper, an efficient implementation scheme for the stabilized index-2 formulation was introduced that requires in each time step the solution of a system of $k + 2m$ nonlinear equations to get $\mathbf{\Delta q}_n, \boldsymbol{\eta}_n, \boldsymbol{\lambda}_{n+1}$.

(b) For equations of motion (1) in linear spaces, the combination of index reduction and generalized-α time integration has been studied by several authors before [26,29,40].

(c) It may be verified straightforwardly that matrix $\mathbf{T}$ in Theorem 2 has three distinct real eigenvalues if $(1-\gamma)/\gamma \neq \alpha_f/(1-\alpha_f)$ and conditions (12) and (50) are satisfied. For parameters according to [14] with $\rho_\infty \in [0, 1)$, all eigenvalues of $\mathbf{T}$ are different and the matrix may be diagonalized. Therefore, $\|\mathbf{T}^n\|$ may be bounded by $C(\varrho(\mathbf{T}))^n$ with a constant C of moderate size and

$$\varrho(\mathbf{T}) = \max\left\{\left|\frac{2\rho_\infty - 1}{2-\rho_\infty}\right|,\ \left|\frac{3\rho_\infty - 1}{3-\rho_\infty}\right|,\ |\rho_\infty|\right\} < 1.$$

In contrast to the original index-3 formulation we observe no substantial amplification of initial errors $\mathbf{E}_0^{\mathbf{z}}$ in time integration.

5 Numerical tests

The motion of a rotating heavy top under the influence of gravity is one of the basic benchmark problems for Lie group time integration methods in multibody dynamics

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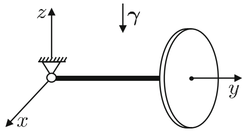

$$m\ddot{\mathbf{x}} - \boldsymbol{\lambda} = m\boldsymbol{\gamma}\,, \qquad (62a)$$
$$\mathbf{J}\dot{\boldsymbol{\Omega}} + \boldsymbol{\Omega} \times \mathbf{J}\boldsymbol{\Omega} + \widetilde{\mathbf{X}}\mathbf{R}^\top\boldsymbol{\lambda} = \mathbf{0}\,, \qquad (62b)$$
$$-\mathbf{x} + \mathbf{R}\mathbf{X} = \mathbf{0}\,. \qquad (62c)$$

Fig. 2 Benchmark problem heavy top [9], see also [19]

[19]. In the present section, we consider a top rotating about a fixed point and its equations of motion in an absolute coordinate formulation, see Fig. 2 and Eq. (62).

In (62), the vector $\mathbf{x}$ represents the position of the center of mass in the inertial frame and $\mathbf{X}$ denotes the position of the center of mass in the body-fixed frame. The orientation of the top is represented by matrix $\mathbf{R} \in SO(3)$. The mass of the top is m, the inertia tensor $\mathbf{J}$ is defined with respect to the center of mass. In the equations of motion (62), there are three algebraic constraints with the associated 3×1 vector $\boldsymbol{\lambda}$ of Lagrange multipliers.

$$m\ddot{\mathbf{x}} - \boldsymbol{\lambda} = m\boldsymbol{\gamma}, \qquad (62a)$$

$$\mathbf{J}\dot{\boldsymbol{\Omega}} + \boldsymbol{\Omega} \times \mathbf{J}\boldsymbol{\Omega} + \widetilde{\mathbf{X}}\mathbf{R}^\top\boldsymbol{\lambda} = \mathbf{0}, \qquad (62b)$$

$$-\mathbf{x} + \mathbf{R}\mathbf{X} = \mathbf{0}. \qquad (62c)$$

The set $\mathbb{R}^3 \times SO(3)$ 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 $G \subset \mathbb{R}^{12}$. The exponential map combines a translation in $\mathbb{R}^3$ and the matrix exponential in SO(3) for the rotation variables that may be evaluated efficiently by the Rodrigues formula, see [9]. Due to the constraints, the motion is restricted to a 3-dimensional submanifold of G and we have

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

Omitting again 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 initial values are set to $\mathbf{R}(0) = \mathbf{I}_3$ and $\boldsymbol{\Omega}(0) = (0,\ 150,\ -4.61538)^\top$. Figure 3 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 using the small time step size $h = 2.5 \times 10^{-5}$.

The numerical test results are in very good agreement with the results of the convergence analysis in Theorems 1 and 2. The left plot of Fig. 4 shows the transient behaviour of Lagrange multiplier $\lambda_3(t)$ for the generalized-α method (9) with step size $h = 1.0 \times 10^{-3}$, parameters $\alpha_m, \alpha_f, \beta, \gamma$ according to (52) and the most straightforward choice of starting values $q_0 = q(t_0)$, $\mathbf{v}_0 = \mathbf{v}(t_0)$, $\dot{\mathbf{v}}_0 = \dot{\mathbf{v}}(t_0)$, $\mathbf{a}_0 = \dot{\mathbf{v}}(t_0)$, $\boldsymbol{\lambda}_0 = \boldsymbol{\lambda}(t_0)$.

For $\rho_\infty = 0.9$, we get very large errors and spurious oscillations in the transient phase that are very similar to the ones that were observed for the mathemat-

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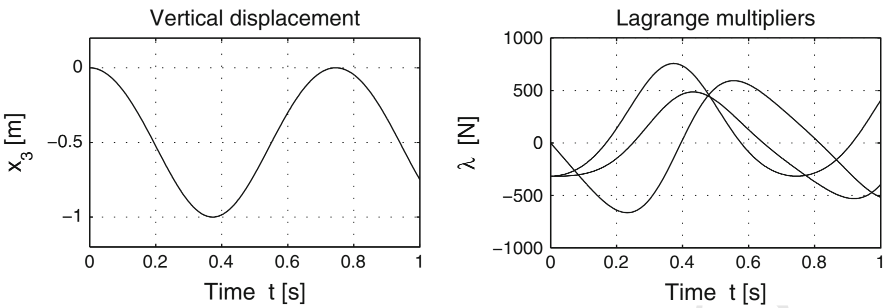

Fig. 3 Benchmark heavy top: reference solution, computed with $h = 2.5 \times 10^{-5}$

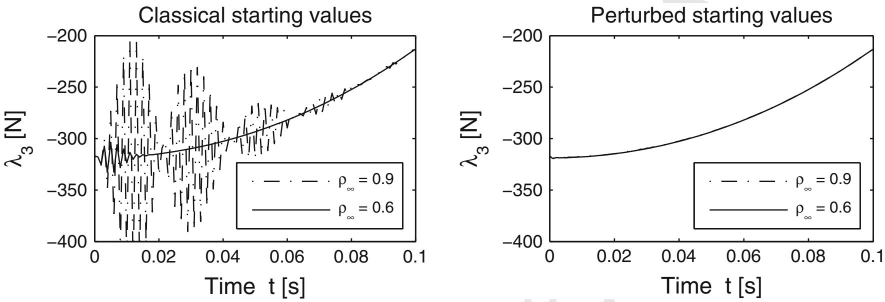

Fig. 4 Index-3 formulation: transient behaviour of λ_3 for time step size $h = 1.0 \times 10^{-3}$

ical pendulum with $x_0 = 0.2$ in Fig. 1. With $\rho_\infty = 0.6$, the numerical damping of the generalized-α method is increased [14]. In the application to constrained systems (1), the spurious oscillations are damped out more rapidly and their maximum amplitude is decreased substantially. The maximum amplitudes are reached at $t = t_{15}$ for $\rho_\infty = 0.9$ and at $t = t_4$ for $\rho_\infty = 0.6$ which corresponds very nicely to $\max_n \|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\| = \|(\mathbf{T}_+^{-1}\mathbf{T}_0)^{14}\| = 34.3$ in the case $\rho_\infty = 0.9$ and to $\max_n \|(\mathbf{T}_+^{-1}\mathbf{T}_0)^n\| = \|(\mathbf{T}_+^{-1}\mathbf{T}_0)^3\| = 7.4$ for $\rho_\infty = 0.6$, see Sect. 4.1.

For perturbed starting values $\mathbf{v}_0$ and $\mathbf{a}_0$ according to (56) and (57), the spurious oscillations disappear and the test results coincide with the reference solution up to plot accuracy, see the right plot of Fig. 4. In these numerical tests, the second order difference approximation $\ddot{\mathbf{v}}_0 \approx (\dot{\mathbf{v}}(t_0 + h) - \dot{\mathbf{v}}(t_0 - h))/(2h)$ was used to evaluate the perturbed starting values $\mathbf{v}_0$, $\mathbf{a}_0$, see Sect. 4.2.

The spurious oscillations may be avoided as well by index reduction. Applying the generalized-α method to the stabilized index-2 formulation of the equations of motion, see Sect. 4.3, the numerical results for $h = 1.0 \times 10^{-3}$ coincide again up to plot accuracy with the reference solution, see the right plot of Fig. 5. The left plot of Fig. 5 shows the time history of the auxiliary variables $\boldsymbol{\eta}$, see (58), for two different time step sizes ($h = 1.0 \times 10^{-3}$ and $h = 5.0 \times 10^{-4}$) illustrating the second order convergence of $\|\mathbf{e}_n^{\boldsymbol{\eta}}\|$ for $h \to 0$.

The large transient errors in the left plot of Fig. 4 do not affect the long-term behaviour of the numerical solution since they are damped out rapidly. Beyond the

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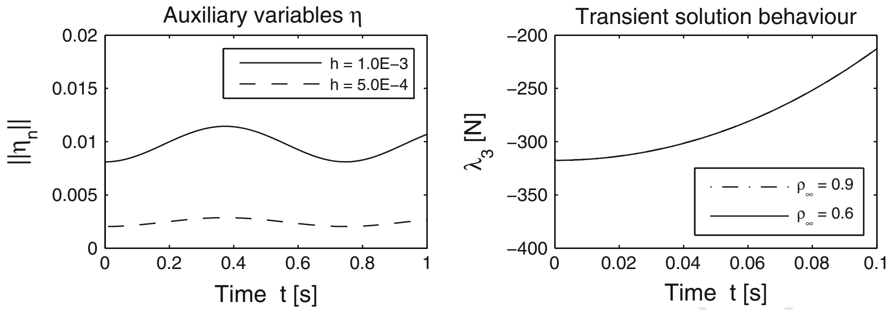

Fig. 5 Stabilized index-2 formulation: $\|\eta_n\|$ vs. $t = t_n$ for two different time step sizes h (*left plot*) and transient behaviour of λ_3 for $h = 1.0 \times 10^{-3}$ (*right plot*)

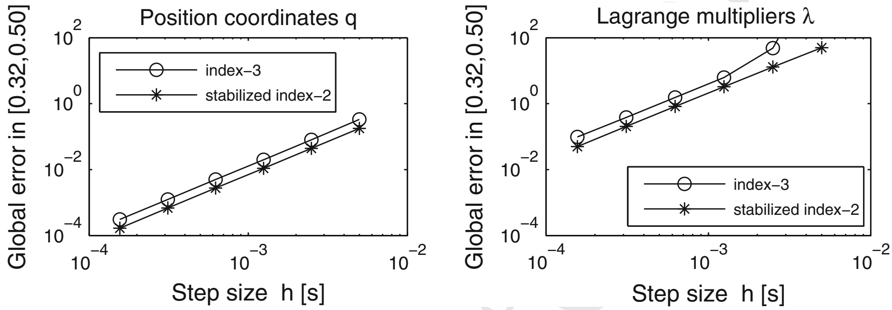

Fig. 6 Maximum global errors $\|\mathbf{e}_n^q\|$, $\|\mathbf{e}_n^\lambda\|$ beyond the transient phase

transient phase, the classical convergence behaviour of a second order time integration method is observed for all solution components, see Fig. 6 and related results from our previous work [3,4,8–10].

For smaller time step sizes h, it is mandatory to scale the systems of linear equations in the corrector iteration appropriately [6,10]. Furthermore, very fine tolerances for absolute and relative errors are used in the stopping criterion of the corrector iteration to guarantee that the constraint residuals $\mathbf{\Phi}(q_{n+1})$ in (9f) and the corresponding error term θ/h^2 in (54) do not affect the result accuracy (ATOL $= 1.0 \times 10^{-12}$, RTOL $= 1.0 \times 10^{-8}$). Increasing these tolerances by a factor of 100, the numerical effort and the computing time may be substantially reduced but for time step sizes $h < 2.0 \times 10^{-4}$ the errors $\|\mathbf{e}_n^\lambda\|$ of the index-3 method are about 8 times larger than before.

6 Summary and conclusions

The representation of constrained mechanical systems in configuration spaces with Lie group structure avoids singularities in the parametrization of rotational degrees of freedom. In generalized-α time integration, the nonlinear structure of the configuration space is taken into account by a nonlinear update of position coordinates with increments that are elements of the corresponding Lie algebra.

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For the convergence analysis, the local and global errors for the position coordinates are defined as elements of the Lie algebra and the Baker–Campbell–Hausdorff formula is applied repeatedly to get an error recursion in a linear space. The coupled error propagation in differential and algebraic solution components is analysed by a rather complex one-step recursion showing that large transient errors are damped out rapidly and second order convergence may be achieved if the method satisfies a set of stability and order conditions.

In the direct application to the index-3 formulation of the equations of motion, the method shows a strange behaviour in the transient phase with spurious oscillations of large amplitude. These oscillations in the Lagrange multipliers may be characterized by an initial error vector of reduced order and by powers of an error amplification matrix that has its spectrum inside the unit circle but a Jordan form with one 3×3 Jordan block resulting in rapidly growing errors in the initial phase.

The order reduction may be avoided adding perturbations of size $\mathcal{O}(h^2)$ to the starting values for velocity and acceleration coordinates. Alternatively, the index of the equations of motion may be reduced before time discretization. The stabilized index-2 formulation combines the original constraints at the level of position coordinates with the hidden constraints at velocity level. The generalized-α Lie group methods are modified to consider in each time step both sets of constraints. The convergence analysis shows, that these modified methods do not suffer from order reduction. Second order convergence may again be proved if stability and order conditions are satisfied.

Similar modifications are necessary to avoid spurious oscillations in variable step size implementations that are subject of further research.

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