The 5th Joint International Conference on Multibody System Dynamics
June 24 – 28, 2018, Lisboa, Portugal

BLieDF2nd - a k-step BDF integrator for constrained mechanical systems on Lie groups

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ABSTRACT — *Multistep methods of BDF type are the methods-of-choice in many industrial multibody system simulation packages. To describe large rotations without singularities, matrix Lie groups are used in this paper. In this framework, BLieDF2nd is a k-step Lie group integrator for second order systems, that avoids order reduction by a slightly perturbed argument of the exponential map for representing the nonlinearity of the numerical flow in the configuration space without any time-consuming re-parametrization. For constrained systems, BLieDF2nd is combined with the index-3 formulation of the equations of motion. For $k \leq 4$, we prove local truncation errors of order $p = k+1$ and convergence of order $p = k$ in all solution components and illustrate the theoretical investigations by numerical tests for the Heavy top benchmark problem in the Lie group formulations $SO(3)$ and $\mathbb{R}^3 \times SO(3)$.*

1 Introduction

Configuration spaces with Lie group structure address the inherent nonlinearity of multibody system models with large rotations. Brüls and Cardona [1] have shown how to avoid time-consuming re-parametrizations of the Lie group in generalized-α time integration. After a short transient phase, the Lie group generalized-α method achieves global second-order accuracy for unconstrained as well as for constrained systems [2]. It may be implemented efficiently following a *Lie algebra approach* [1, 3], that substitutes traditional updates of configuration variables in the (*nonlinear*) Lie group by updates of solution increments in a *linear* space.

In the present paper, we discuss the extension of this approach to multistep methods of BDF type which were first developed by Curtiss and Hirschfelder [4] for the numerical integration of ordinary differential equations. They became famous for solving stiff differential equations by the work of Gear [5]. Now they are the methods-of-choice in many industrial multibody system simulation packages [6]. In 2001, Faltinsen et al. [7] extended multistep methods (including the BDF methods) to the Lie group setting. In this paper the integrator BLieDF2nd for second order systems on Lie groups is introduced, which avoids frequent evaluations of the inverse exponential map beyond the initialization phase and needs only one matrix commutator calculation per step for $k \leq 4$, which makes it computationally more efficient than the Lie group multistep methods of Faltinsen et al. [7].

The remaining part of the paper is organized as follows: In Section 1.1 and 1.2, we introduce an increment notation for BDF in linear spaces. In Section 2, this approach is extended to the equations of motion in configuration spaces with Lie group structure. The basic steps of local and global error analysis are sketched in Section 3. In Section 4, the results of this convergence analysis are illustrated by numerical tests for a classical benchmark problem.

1.1 BDF methods for first order ODEs

The multistep BDF methods were originally introduced to solve ordinary differential equations

$$\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}) \tag{1}$$

with $\mathbf{x} : \mathbb{R} \to \mathbb{R}^n$ and $\mathbf{f} : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$. For the time step $t_n \to t_{n+1} = t_n + h$ the k-step fixed step size BDF method is given by

$$\frac{1}{h}\sum_{i=0}^{k} \alpha_i \mathbf{x}_{n+1-i} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}), \tag{2}$$

such that α_i for $i = 0, \ldots, k$ fulfil the order conditions

$$\sum_{i=0}^{k} \alpha_i = 0 \text{ and } \sum_{i=0}^{k} \alpha_i \frac{(k-i)^l}{k^{l-1}} = l,\ (l = 1, \ldots, k) \tag{3}$$

to get local truncation errors of size $\mathscr{O}(h^{k+1})$, see [8]. For $k = 2,\ 3,\ 4$ these parameters are given by

$$\begin{aligned}
k = 2: &\qquad \alpha_0 = \frac{3}{2},\ \alpha_1 = -2,\ \alpha_2 = \frac{1}{2}, \\
k = 3: &\qquad \alpha_0 = \frac{11}{6},\ \alpha_1 = -3,\ \alpha_2 = \frac{3}{2},\ \alpha_3 = -\frac{1}{3}, \\
k = 4: &\qquad \alpha_0 = \frac{25}{12},\ \alpha_1 = -4,\ \alpha_2 = 3,\ \alpha_3 = -\frac{4}{3},\ \alpha_4 = \frac{1}{4}.
\end{aligned}$$

By introducing new parameters

$$\gamma_i := \sum_{j=0}^{i-1} \alpha_j,\ (i = 1, \ldots, k), \tag{5}$$

given by

$$\begin{aligned}
k = 2: &\qquad \gamma_1 = \frac{3}{2},\ \gamma_2 = -\frac{1}{2}, \\
k = 3: &\qquad \gamma_1 = \frac{11}{6},\ \gamma_2 = -\frac{7}{6},\ \gamma_3 = \frac{1}{3}, \\
k = 4: &\qquad \gamma_1 = \frac{25}{12},\ \gamma_2 = -\frac{23}{12},\ \gamma_3 = \frac{13}{12},\ \gamma_4 = -\frac{1}{4},
\end{aligned}$$

equation (2) may be rewritten as

$$\sum_{i=1}^{k} \gamma_i \frac{\mathbf{x}_{n+2-i} - \mathbf{x}_{n+1-i}}{h} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1})$$

with order conditions

$$\sum_{i=1}^{k} \gamma_i \frac{(k+1-i)^l - (k-i)^l}{k^{l-1}} = l,\ (l = 1, \ldots, k) \tag{7}$$

that follow directly from (3) and (5). For given vectors $\mathbf{x}_{n+1-i}$, $(i = 1, \ldots, k)$, variables

$$\boldsymbol{\Delta}\mathbf{x}_{n+1-i} := \frac{\mathbf{x}_{n+2-i} - \mathbf{x}_{n+1-i}}{h},\ (i = 2, \ldots, k)$$

can be defined to obtain the numerical solution $\mathbf{x}_{n+1} \approx \mathbf{x}(t_{n+1})$ by the one-step update $\mathbf{x}_{n+1} = \mathbf{x}_n + h\boldsymbol{\Delta}\mathbf{x}_n$ with a vector $\boldsymbol{\Delta}\mathbf{x}_n$ that is obtained solving the corrector equations

$$\sum_{i=1}^{k} \gamma_i \boldsymbol{\Delta}\mathbf{x}_{n+1-i} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}). \tag{8}$$

1.2 BDF methods for second order ODEs

The second order ODE

$$\mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} = -\mathbf{g}(t,\mathbf{q},\dot{\mathbf{q}}) \tag{9}$$

with position coordinate $\mathbf{q} : \mathbb{R} \to \mathbb{R}^n$, mass matrix $\mathbf{M}$ and force vector $\mathbf{g}$ is considered in its equivalent first order form

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{v}, \\ \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= -\mathbf{g}(t,\mathbf{q},\mathbf{v}) \end{aligned}$$

with velocity vector $\mathbf{v} \in \mathbb{R}^n$. For second order ODEs, the time step $t_n \to t_{n+1} = t_n + h$ of the BDF method for first order ODEs (8) can be rewritten as

$$\mathbf{q}_{n+1} = \mathbf{q}_n + h\boldsymbol{\Delta}\mathbf{q}_n, \tag{11a}$$

$$\sum_{i=1}^{k} \gamma_i \boldsymbol{\Delta}\mathbf{q}_{n+1-i} = \mathbf{v}_{n+1}, \tag{11b}$$

$$\frac{1}{h}\mathbf{M}(\mathbf{q}_{n+1})\sum_{i=0}^{k} \alpha_i \mathbf{v}_{n+1-i} = -\mathbf{g}(t_{n+1},\mathbf{q}_{n+1},\mathbf{v}_{n+1}) \tag{11c}$$

by using the vectors

$$\mathbf{q}_n,\ \boldsymbol{\Delta}\mathbf{q}_{n+1-i},\ (i=2,...,k),\ \mathbf{v}_{n+1-i},\ (i=1,...,k)$$

to get numerical solutions $\mathbf{q}_{n+1} \approx \mathbf{q}(t_{n+1})$, $\boldsymbol{\Delta}\mathbf{q}_{n+1} \approx \dot{\mathbf{q}}(t_{n+1})$, $\mathbf{v}_{n+1} \approx \mathbf{v}(t_{n+1})$. In the very first time step the k-step BDF method (11) is initialized by

$$\mathbf{q}_{k-1} \approx \mathbf{q}(t_{k-1}),\ \boldsymbol{\Delta}\mathbf{q}_j \approx \frac{\mathbf{q}(t_{j+1}) - \mathbf{q}(t_j)}{h},\ (j=0,...,k-2),\ \mathbf{v}_j \approx \mathbf{v}(t_j),\ (j=0,...,k-1). \tag{12}$$

Note, that (11) with initialization scheme (12) defines exactly the same numerical solutions $(\mathbf{q}_n, \mathbf{v}_n)$ as the classical BDF (2) for the first order system (1). Therefore, the method is zero-stable for $1 \le k \le 6$ and has order of convergence $p = k$. For $k \le 2$, the method is A-stable and for $3 \le k \le 6$ there is A-stability, see [8, 9].

2 BDF for mechanical systems on Lie groups

Following the approach of Brüls and Cardona [1], the ODE integrator (11) with its one-step update (11a) for the configuration variables $\mathbf{q}$ is applied in a slightly modified form to mechanical systems that have nonlinear configuration spaces with Lie group structure. Theoretical and practical aspects of such Lie group integrators have been discussed in great detail for the generalized-α Lie group method [1, 2, 3, 10].
In the present paper, a k-step BDF Lie group integrator for 2nd order systems is constructed, the BLieDF2$^{\text{nd}}$, that shares most of favourable properties of the approach of Brüls and Cardona [1] and is computationally more efficient than the Lie group multistep method of Faltinsen et al. [7], since it avoids frequent evaluations of the inverse of the derivative of the exponential map and needs less calculations of the matrix commutator. The main interest is the proposed BLieDF2$^{\text{nd}}$ integrator for $2 \le k \le 4$. For methods with $k \ge 5$ (that are less interesting from the practical viewpoint) there is a risk of order reduction.

2.1 Matrix Lie groups

An m-dimensional Lie group G is a differentiable manifold, with a neutral element $e \in G$ and two differentiable mappings. The first one is the group operation $\circ : G \times G \mapsto G$ and the second one an inverse map, see [11]. In this paper, subgroups of the general linear space $GL(n)$, the so-called matrix Lie groups, are considered. The Lie groups

$SO(3) := \{\mathbf{R} \in \mathbb{R}^{3\times 3} : \mathbf{R}^T\mathbf{R} = \mathbf{I}_3,\ \det\mathbf{R} = 1\}$, which is the special orthogonal group and $\mathbb{R}^3 \times SO(3)$ are examined. The group operation for two rotation matrices $\mathbf{R}$ of the first Lie group is given by the matrix multiplication

$$\mathbf{R}_1 \circ \mathbf{R}_2 = \mathbf{R}_1\mathbf{R}_2 \text{ with } \mathbf{R}_1, \mathbf{R}_2 \in SO(3).$$

An element q of the Lie group $\mathbb{R}^3 \times SO(3)$ is a pair $q = (\mathbf{x}, \mathbf{R})$ with the translation vector $\mathbf{x} \in \mathbb{R}^3$ and the rotation matrix $\mathbf{R} \in SO(3)$. The group operation is defined by

$$(\mathbf{x}_1, \mathbf{R}_1) \circ (\mathbf{x}_2, \mathbf{R}_2) \quad = \quad (\mathbf{x}_1 + \mathbf{x}_2, \mathbf{R}_1\mathbf{R}_2), \text{ with } \mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^3,\ \mathbf{R}_1, \mathbf{R}_2 \in SO(3).$$

The configuration of a rigid body at time t can be described by a function $q(t) :\ [t_0, t_{\text{end}}] \to\ G$. For a differential equation on a Lie group G the equivalence

$$q(t) \in G \ \Leftrightarrow\ \dot{q}(t) \in T_{q(t)}G,\ (t \in [t_0, t_{\text{end}}]) \text{ with } q(t_0) \in G$$

is valid, where $T_{q(t)}G$ is the tangent space of G at $q(t)$. An important tangent space is the Lie algebra $\mathfrak{g} := T_eG$, which is isomorphic to $\mathbb{R}^m$ by a map $\widetilde{(\bullet)} :\ \mathbb{R}^m \to \mathfrak{g}$. For matrix Lie groups, the matrix commutator

$$[\mathbf{A}, \mathbf{B}] := \mathbf{AB} - \mathbf{BA} \text{ with } \mathbf{A}, \mathbf{B} \in \mathfrak{g} \tag{13}$$

is defined. For $G = \mathbb{R}^3 \times SO(3)$, an element $\widetilde{\mathbf{v}} \in \mathfrak{g}$ can be separated in two variables by $\mathbf{v} = (\mathbf{u}^T, \boldsymbol{\Omega}^T)^T$ with the translation velocity $\mathbf{u}$ in the inertial frame and the angular velocity $\boldsymbol{\Omega}$ in the body-attached frame. By means of the exponential map $\exp : \mathfrak{g} \to G$ with

$$\exp(\widetilde{\mathbf{v}}) = \sum_{i=0}^{\infty} \frac{1}{i!}\widetilde{\mathbf{v}}^i \tag{14}$$

an element of the Lie algebra is mapped to the Lie group. Furthermore, a linear operator $\widehat{(\bullet)} : \mathbb{R}^m \to \mathbb{R}^{m\times m},\ \mathbf{v} \mapsto \widehat{\mathbf{v}}$ is defined by

$$\widetilde{\widehat{\mathbf{v}}\mathbf{w}} = [\widetilde{\mathbf{v}}, \widetilde{\mathbf{w}}] \text{ for all } \mathbf{w} \in \mathbb{R}^m. \tag{15}$$

2.2 Equations of motion

In this paper, BLieDF2$^{\text{nd}}$ is applied to unconstrained and constrained mechanical systems on Lie groups. In the unconstrained case, the equations of motion for Lie group formulations are given by

$$\dot{q} \quad = \quad DL_q(e) \cdot \widetilde{\mathbf{v}}, \tag{16a}$$
$$\mathbf{M}(q)\dot{\mathbf{v}} \quad = \quad -\mathbf{g}(q, \mathbf{v}, t) \tag{16b}$$

with position coordinates $q \in G$, velocity coordinates $\mathbf{v} \in \mathbb{R}^m$, mass matrix $\mathbf{M}(q)$, that should be symmetric, positive definite and force vector $\mathbf{g}(q, \mathbf{v}, t)$. The directional derivative $DL_q(e) :\ \mathfrak{g} \to\ T_qG,\ \widetilde{\mathbf{v}} \mapsto\ DL_q(e) \cdot \widetilde{\mathbf{v}}$ of the left translation $L_q(y)$ in $y = e$ along $\widetilde{\mathbf{v}}$ is used to summarize the kinematic relations in their compact form (16a) instead of (11a) for the second order ODE (9), see [1].
To extend the method to constrained mechanical systems, the equations of motion are examined as differential-algebraic equations in the index-3 formulation (17), see [1]

$$\dot{q} \quad = \quad DL_q(e) \cdot \widetilde{\mathbf{v}}, \tag{17a}$$
$$\mathbf{M}(q)\dot{\mathbf{v}} \quad = \quad -\mathbf{g}(q, \mathbf{v}, t) - \mathbf{B}^T(q)\boldsymbol{\lambda}, \tag{17b}$$
$$\mathbf{0} \quad = \quad \boldsymbol{\Phi}(q) \tag{17c}$$

with $l \leq m$ linearly independent holonomic constraints (17c), constraint gradients $\mathbf{B}(q)$ with

$$D\boldsymbol{\Phi}(q) \cdot (DL_q(e) \cdot \widetilde{\mathbf{w}}) = \mathbf{B}(q)\mathbf{w},\ (\mathbf{w} \in \mathbb{R}^m), \tag{18}$$

and Lagrange multipliers $\boldsymbol{\lambda} \in \mathbb{R}^l$. The hidden constraints at velocity level can be obtained by differentiating equation (17c) with respect to t

$$\mathbf{0} = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{\Phi}(q(t)) = \mathrm{D}\mathbf{\Phi}(q(t))\cdot\dot{q}(t) = \mathrm{D}\mathbf{\Phi}(q(t))\cdot(\mathrm{D}L_q(e)\cdot\widetilde{\mathbf{v}}) = \mathbf{B}(q)\mathbf{v}.$$

Furthermore, the derivative of $\mathbf{\Theta}(q,\mathbf{w}) := \mathbf{B}(q)\mathbf{w}$ with respect to q may be represented by

$$D_q\mathbf{\Theta}(q,\mathbf{w})\cdot(DL_q(e)\cdot\widetilde{\mathbf{z}}) = \mathbf{Z}(q)(\mathbf{w},\mathbf{z}) \text{ for all } \mathbf{w},\mathbf{z}\in\mathbb{R}^m \tag{19}$$

with a bilinear form $\mathbf{Z}(q) : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^l$.

2.3 BDF for unconstrained mechanical systems on Lie groups

To apply the BDF method for second order ODEs (11) in Lie group formulation, the one-step update (11a) is replaced by (see [1]),

$$q_{n+1} = q_n \circ \exp(h\widetilde{\mathbf{\Delta q}_n}).$$

In that way, the BDF time step $t_n \to t_{n+1}$ in the Lie group G is expressed in terms of an element $\widetilde{\mathbf{\Delta q}_n} \in \mathfrak{g}$ and the method may be written similar to (11) with increments $\widetilde{\mathbf{\Delta q}}_{n+1-i}$ in the Lie algebra.
The k-step BLieDF2$^{\text{nd}}$ for time step $t_n \to t_{n+1} = t_n + h$ updates the numerical solutions according to

$$\begin{aligned} q_{n+1} &= q_n \circ \exp(h\widetilde{\mathbf{\Delta q}_n}), && (20a)\\ \sum_{i=1}^{k}\gamma_i \mathbf{\Delta q}_{n+1-i} &= \mathbf{v}_{n+1} + h^2\mathbf{L}_k(\mathbf{v}_n,\mathbf{v}_{n-1},\dots,\mathbf{v}_{n-k+1};h), && (20b)\\ \frac{1}{h}\mathbf{M}(q_{n+1})\sum_{i=0}^{k}\alpha_i\mathbf{v}_{n+1-i} &= -\mathbf{g}(t_{n+1},q_{n+1},\mathbf{v}_{n+1}) && (20c) \end{aligned}$$

starting with

$$q_{k-1} \approx q(t_{k-1}),\ q(t_{j+1}) \approx q(t_j)\circ\exp(h\widetilde{\mathbf{\Delta q}}_j),\ (j=0,...,k-2),\ \mathbf{v}_j \approx \mathbf{v}(t_j),\ (j=0,...,k-1). \tag{21}$$

This initialization scheme requires $k-1$ evaluations of the inverse of the exponential map to get high order approximations $\mathbf{\Delta q}_j$ from $(q(t_j))^{-1}\circ q(t_{j+1})$, $(j=0,...,k-2)$, before the first time step.
Note the correction term $h^2\mathbf{L}_k(\mathbf{v}_n,\mathbf{v}_{n-1},\dots,\mathbf{v}_{n-k+1};h)$ that was inserted to avoid order reduction and is identically zero in linear spaces, see (11). Without this correction term the order of convergence would decrease to $p = \min\{k,2\}$ in the Lie group setting, see Section 4.2. Guided by the convergence analysis, this term can be defined by

$$\begin{aligned} \mathbf{L}_2 &\equiv \mathbf{0}, && (22a)\\ \mathbf{L}_3 &= \mathbf{L}_3(\mathbf{v}_n,\mathbf{v}_{n-1},\mathbf{v}_{n-2};h) := \tfrac{1}{12}\widehat{\mathbf{v}}_n\dot{\mathbf{v}}_n \quad \text{with } \dot{\mathbf{v}}_n := \frac{3\mathbf{v}_n - 4\mathbf{v}_{n-1} + \mathbf{v}_{n-2}}{2h}, && (22b)\\ \mathbf{L}_4 &= \mathbf{L}_4(\mathbf{v}_n,\mathbf{v}_{n-1},\mathbf{v}_{n-2},\mathbf{v}_{n-3};h) := \tfrac{1}{12}\widehat{\mathbf{v}}_n\dot{\mathbf{v}}_{n+1} \quad \text{with } \dot{\mathbf{v}}_{n+1} := \frac{7\mathbf{v}_n - 7\mathbf{v}_{n-1} - 3\mathbf{v}_{n-2} + 3\mathbf{v}_{n-3}}{4h} && (22c) \end{aligned}$$

with the operator $\widehat{(\bullet)}$ from (15). The approximations of $\dot{\mathbf{v}}_n$ and $\dot{\mathbf{v}}_{n+1}$ are not fixed and can be substituted by another difference approximation of appropriate order.

2.4 BDF for constrained mechanical systems on Lie groups

For applying the BLieDF2$^{\text{nd}}$ (20) to constrained systems (17), the holonomic constraints (17c), as well as the auxiliary variables $\boldsymbol{\lambda}$, need to be added.

The time step $t_n \to t_{n+1} = t_n + h$ for the k-step BLieDF2$^{\text{nd}}$ for constrained systems in the index-3 formulation (17) is given by

$$
\begin{aligned}
q_{n+1} &= q_n \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}_n}), && (23a)\\
\sum_{i=1}^{k} \gamma_i \boldsymbol{\Delta}\mathbf{q}_{n+1-i} &= \mathbf{v}_{n+1} + h^2 \mathbf{L}_k(\mathbf{v}_n, \mathbf{v}_{n-1}, \ldots, \mathbf{v}_{n-k+1}; h), && (23b)\\
\frac{1}{h}\mathbf{M}(q_{n+1}) \sum_{i=0}^{k} \alpha_i \mathbf{v}_{n+1-i} &= -\mathbf{g}(t_{n+1}, q_{n+1}, \mathbf{v}_{n+1}) - \mathbf{B}^T(q_{n+1})\boldsymbol{\lambda}_{n+1}, && (23c)\\
\boldsymbol{\Phi}(q_{n+1}) &= \mathbf{0} && (23d)
\end{aligned}
$$

with initialization according to (21) and correction term (22).

3 Error analysis

3.1 Local truncation errors

For unconstrained systems in linear spaces, the local errors of a k-step BDF method are of order $p = k+1$, see [8]. For configuration spaces with Lie group structure the calculation of local truncation errors is more complicated. Because of the exponential map (14) in the update formulas (20a) and (23a), the Baker-Campbell-Hausdorff formula (see [11]) must be applied in the analysis. Therefore, we obtain local errors that include matrix commutators (13) that vanish in linear spaces.
The local truncation errors $\mathbf{l}_n^q$, $\mathbf{l}_n^{\mathbf{v}}$ are defined by inserting the analytical solution into the BLieDF2$^{\text{nd}}$ update formulae:

$$
\begin{aligned}
\sum_{i=1}^{k} \gamma_i \boldsymbol{\Delta}\mathbf{q}(t_{n+1-i}) &= \mathbf{v}(t_{n+1}) + h^2 \mathbf{L}_k(\mathbf{v}(t_n), \mathbf{v}(t_{n-1}), \ldots, \mathbf{v}(t_{n-k+1}); h) + \frac{\mathbf{l}_n^q}{h}, && (24a)\\
\frac{1}{h}\mathbf{M}(q(t_{n+1})) \sum_{i=0}^{k} \alpha_i \mathbf{v}(t_{n+1-i}) &= -\mathbf{g}(t_{n+1}, q(t_{n+1}), \mathbf{v}(t_{n+1})) - \mathbf{B}^T(q(t_{n+1}))\boldsymbol{\lambda}(t_{n+1}) + \frac{\mathbf{l}_n^{\mathbf{v}}}{h}. && (24b)
\end{aligned}
$$

Here, we use a function $\boldsymbol{\Delta}\mathbf{q} : [t_0, t_{\text{end}}] \to \mathbb{R}^m$ being implicitly defined by

$$
q(t+h) = q(t) \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t)). \tag{25}
$$

At first the correction term $\mathbf{L}_k$ from (22) is examined for analytical solutions $\mathbf{v}(t_n)$.
Lemma 1: For $2 \le k \le 4$ the correction term (22) satisfies

$$
\begin{aligned}
\mathbf{L}_2(\mathbf{v}(t_n), \mathbf{v}(t_{n-1})) &= \mathbf{0}, && (26a)\\
\mathbf{L}_3(\mathbf{v}(t_n), \mathbf{v}(t_{n-1}), \mathbf{v}(t_{n-2})) &= \frac{1}{12}\widehat{\mathbf{v}}(t_n)\dot{\mathbf{v}}(t_n) + \mathscr{O}(h), && (26b)\\
\mathbf{L}_4(\mathbf{v}(t_n), \mathbf{v}(t_{n-1}), \mathbf{v}(t_{n-2}), \mathbf{v}(t_{n-3})) &= \frac{1}{12}\widehat{\mathbf{v}}(t_n)(\dot{\mathbf{v}}(t_n) + h\ddot{\mathbf{v}}(t_n)) + \mathscr{O}(h^2). && (26c)
\end{aligned}
$$

Proof: For $k = 2$ the assertion is trivial, since $\mathbf{L}_2 \equiv \mathbf{0}$. For $k = 3$ and $k = 4$, Taylor expansion is used to show

$$
\begin{aligned}
\mathbf{L}_3(\mathbf{v}(t_n), \mathbf{v}(t_{n-1}), \mathbf{v}(t_{n-2})) &= \frac{1}{12}\widehat{\mathbf{v}}(t_n)\frac{3\mathbf{v}(t_n) - 4\mathbf{v}(t_{n-1}) + \mathbf{v}(t_{n-2})}{2h}\\
&= \frac{1}{12}\widehat{\mathbf{v}}(t_n)\frac{3\mathbf{v}(t_n) - 4(\mathbf{v}(t_n) - h\dot{\mathbf{v}}(t_n)) + \mathbf{v}(t_n) - 2h\dot{\mathbf{v}}(t_n)}{2h} + \mathscr{O}(h)\\
&= \frac{1}{12}\widehat{\mathbf{v}}(t_n)\dot{\mathbf{v}}(t_n) + \mathscr{O}(h)
\end{aligned}
$$

and

$$
\begin{aligned}
\mathbf{L}_4(\mathbf{v}(t_n),\mathbf{v}(t_{n-1}),\mathbf{v}(t_{n-2}),\mathbf{v}(t_{n-3})) &= \frac{1}{12}\widehat{\mathbf{v}}(t_n)\frac{7\mathbf{v}(t_n)-7\mathbf{v}(t_{n-1})-3\mathbf{v}(t_{n-2})+3\mathbf{v}(t_{n-3})}{4h} \\
&= \frac{1}{12}\widehat{\mathbf{v}}(t_n)(\dot{\mathbf{v}}(t_n)+h\ddot{\mathbf{v}}(t_n))+\mathscr{O}(h^2).
\end{aligned}
$$

■

With Theorem 1 the local truncation errors for the k-step BLieDF2$^{\text{nd}}$ with $k \in \{2,3,4\}$ can be estimated to be of size $\mathscr{O}(h^{k+1})$ for the constrained mechanical systems in Lie group formulation:

Theorem 1: The local truncation errors defined by (24) of the k-step BLieDF2$^{\text{nd}}$ methods, (20) and (23) are of size

$$
\mathbf{l}_n^q = \mathscr{O}(h^{k+1}),\ \frac{\mathbf{l}_{n+1}^q-\mathbf{l}_n^q}{h} = \mathscr{O}(h^{k+1}) \text{ and } \mathbf{l}_n^{\mathbf{v}} = \mathscr{O}(h^{k+1}) \tag{27}
$$

for $2 \le k \le 4$ if the order conditions (3) or (7) are fulfilled.

Proof:

a) At first, the local error $\mathbf{l}_n^q$ is examined. As a result of the Magnus series expansion, the flow of $\dot{q}(t) = DL_q(e)\cdot\widetilde{\mathbf{v}}(t)$ with a smooth function $\mathbf{v}(t)$ can be locally represented by

$$
q(t+h) = q(t)\circ\exp(h\widetilde{\boldsymbol{\nu}}(h;t,\mathbf{v}(t))) \tag{28}
$$

with a smooth function $\widetilde{\boldsymbol{\nu}} : [-h_0,h_0]\times\mathbb{R}\times G \to \mathfrak{g}$ that satisfies

$$
h\widetilde{\boldsymbol{\nu}}(h;t,\mathbf{v}(t)) = h\widetilde{\mathbf{v}}(t)+\frac{h^2}{2}\dot{\widetilde{\mathbf{v}}}(t)+\frac{h^3}{6}\ddot{\widetilde{\mathbf{v}}}(t)+\frac{h^3}{12}[\widetilde{\mathbf{v}}(t),\dot{\widetilde{\mathbf{v}}}(t)]+\frac{h^4}{24}\dddot{\widetilde{\mathbf{v}}}(t)+\frac{h^4}{24}[\widetilde{\mathbf{v}}(t),\ddot{\widetilde{\mathbf{v}}}(t)]+\mathscr{O}(h^5), \tag{29}
$$

see [11], [12]. Note, that the matrix commutators in (29) vanish identically in linear spaces since the arguments commute in this case. The comparison of (25) and (28) shows $\boldsymbol{\Delta}\mathbf{q}(t_{n+1-i}) = \boldsymbol{\nu}(h;t_{n+1-i},\mathbf{v}(t_{n+1-i}))$, $(i=1,...,k)$, with $t_{n+1-i} \ = \ t_n+(1-i)h$. Taylor expansion yields

$$
\begin{aligned}
\boldsymbol{\Delta}\mathbf{q}(t_{n+1-i}) &= \mathbf{v}(t_n)+\left(\frac{3}{2}-i\right)h\dot{\mathbf{v}}(t_n)+\left(\frac{7}{6}-\frac{3}{2}i+\frac{1}{2}i^2\right)h^2\ddot{\mathbf{v}}(t_n)+\left(\frac{5}{8}-\frac{7}{6}i+\frac{3}{4}i^2-\frac{1}{6}i^3\right)h^3\dddot{\mathbf{v}}(t_n) \\
&\quad +\frac{1}{12}h^2\widehat{\mathbf{v}}(t_n)\dot{\mathbf{v}}(t_n)+\left(\frac{1}{8}-\frac{1}{12}i\right)h^3\widehat{\mathbf{v}}(t_n)\ddot{\mathbf{v}}(t_n)+\mathscr{O}(h^4).
\end{aligned} \tag{30}
$$

In (24a), the local truncation error $\mathbf{l}_n^q$ is given by

$$
\begin{aligned}
\mathbf{l}_n^q &= h\sum_{i=1}^{k}\gamma_i\boldsymbol{\Delta}\mathbf{q}(t_{n+1-i})-h\mathbf{v}(t_n)-h^2\dot{\mathbf{v}}(t_n)-\frac{h^3}{2}\ddot{\mathbf{v}}(t_n)-\frac{h^4}{6}\dddot{\mathbf{v}}(t_n) \\
&\quad -h^3\mathbf{L}_k(\mathbf{v}(t_n),\mathbf{v}(t_{n-1}),\ldots,\mathbf{v}(t_{n-k+1});h)+\mathscr{O}(h^5).
\end{aligned}
$$

By inserting (30), $\mathbf{l}_n^q$ may be estimated by

$$
\begin{aligned}
\mathbf{l}_n^q &= h\left(\sum_{i=1}^{k}\gamma_i-1\right)\mathbf{v}(t_n)+h^2\left(\sum_{i=1}^{k}\gamma_i\left(\frac{3}{2}-i\right)-1\right)\dot{\mathbf{v}}(t_n)+\frac{h^3}{12}\sum_{i=1}^{k}\gamma_i\widehat{\mathbf{v}}(t_n)\dot{\mathbf{v}}(t_n) \\
&\quad +h^3\left(\sum_{i=1}^{k}\gamma_i\left(\frac{7}{6}-\frac{3}{2}i+\frac{1}{2}i^2\right)-\frac{1}{2}\right)\ddot{\mathbf{v}}(t_n)+h^4\sum_{i=1}^{k}\gamma_i\left(\frac{1}{8}-\frac{1}{12}i\right)\widehat{\mathbf{v}}(t_n)\ddot{\mathbf{v}}(t_n) \\
&\quad +h^4\left(\sum_{i=1}^{k}\gamma_i\left(\frac{5}{8}-\frac{7}{6}i+\frac{3}{4}i^2-\frac{1}{6}i^3\right)-\frac{1}{6}\right)\dddot{\mathbf{v}}(t_n)-h^3\mathbf{L}_k(\mathbf{v}(t_n),\mathbf{v}(t_{n-1}),\ldots,\mathbf{v}(t_{n-k+1});h)+\mathscr{O}(h^5).
\end{aligned}
$$

With Lemma 1 and the order conditions (7) it follows $\mathbf{l}_n^q = \mathscr{O}(h^{k+1})$ if $k \le 4$.

b) Let $\mathbf{l}^q_{n,k}$ be the local error in q of the k-step BLieDF2[nd] for time step $t_n \to t_{n+1}$. From part a) it is known, that this error is given by $\mathbf{l}^q_{n,k} = C_{k+1}h^{k+1}\mathbf{v}^{(k)}(t_n) + h^{k+1}\mathbf{f}(\mathbf{v}(t_n), \dot{\mathbf{v}}(t_n), ..., \mathbf{v}^{(k-1)}(t_n)) + \mathscr{O}(h^{k+2})$ with a function $\mathbf{f}$ that consists of several matrix commutators (13) and a non-zero constant C_{k+1}. Because of that, we have

$$
\begin{aligned}
\frac{\mathbf{l}^q_{n+1,k} - \mathbf{l}^q_{n,k}}{h} &= \frac{C_{k+1}h^{k+1}\mathbf{v}^{(k)}(t_{n+1}) + h^{k+1}\mathbf{f}(\mathbf{v}(t_{n+1}), \dot{\mathbf{v}}(t_{n+1}), ..., \mathbf{v}^{(k-1)}(t_{n+1})) + \mathscr{O}(h^{k+2})}{h} \\
&\quad - \frac{C_{k+1}h^{k+1}\mathbf{v}^{(k)}(t_n) + h^{k+1}\mathbf{f}(\mathbf{v}(t_n), \dot{\mathbf{v}}(t_n), ..., \mathbf{v}^{(k-1)}(t_n)) + \mathscr{O}(h^{k+2})}{h} \\
&= \frac{C_{k+1}h^{k+1}\mathbf{v}^{(k)}(t_n) + h^{k+1}\mathbf{f}(\mathbf{v}(t_n), \dot{\mathbf{v}}(t_n), ..., \mathbf{v}^{(k-1)}(t_n))}{h} \\
&\quad - \frac{C_{k+1}h^{k+1}\mathbf{v}^{(k)}(t_n) + h^{k+1}\mathbf{f}(\mathbf{v}(t_n), \dot{\mathbf{v}}(t_n), ..., \mathbf{v}^{(k-1)}(t_n))}{h} + \mathscr{O}(h^{k+1}) \\
&= \mathscr{O}(h^{k+1}).
\end{aligned}
$$

c) The local error estimate $\mathbf{l}^{\mathbf{v}}_n = \mathscr{O}(h^{k+1})$ follows as for the k-step BDF method in linear spaces, see [8]. ■

This theorem shows for $k \le 4$, that there is the same order of local errors in the k-step BDF methods for constrained mechanical systems in Lie group formulation as for ODEs in linear spaces.

3.2 Global error recursion

A k-step BDF method in linear spaces has the order of convergence $p = k$ if $k \le 6$, see [8]. The aim is to prove this for constrained mechanical systems in Lie group formulation, as well. Taking into account the complex structure of the local error terms in the Lie group case, we focus on the practically relevant methods with $k \le 4$.
The multistep method will be written in terms of a one step method in a higher dimensional configuration space as it is done for the BDF methods in linear spaces, see [8]. For configuration spaces with Lie group structure, the proof is similar to the corresponding convergence analysis for the generalized-α method, see [10].
The global errors are defined by

$$
\begin{aligned}
q(t_n) &= q_n \circ \exp(\widetilde{\mathbf{e}}^q_n), && (31a)\\
\mathbf{\Delta q}(t_n) &= \mathbf{\Delta q}_n + \mathbf{e}^{\mathbf{\Delta q}}_n, && (31b)\\
(\bullet)(t_n) &= (\bullet)_n + \mathbf{e}^{(\bullet)}_n && (31c)
\end{aligned}
$$

with $(\bullet)$ being either $\mathbf{v}$ or $\boldsymbol{\lambda}$. We restrict the convergence analysis to numerical solutions q_n remaining in a neighbourhood of size $\mathscr{O}(h)$ of the analytical solution. Similar to arguments in the proof of Theorem VII.3.5 in [9], we suppose that for all $h \in (0, h_0]$ and all r with $t_0 + rh \in [t_0, t_{\text{end}}]$, there are positive constants h_0 and C such that

$$\|\mathbf{e}^q_r\| \le Ch \tag{32}$$

and we define

$$\varepsilon_n := \|\mathbf{e}^q_n\| + \|\mathbf{e}^{\mathbf{v}}_n\| + h\|\mathbf{e}^{\mathbf{M}^{-1}\mathbf{B}^T\boldsymbol{\lambda}}_n\|$$

to summarize higher order terms. Here, we use the notation $\mathbf{e}^{(\mathbf{C}\bullet)} := \mathbf{C}(q(t_n))\mathbf{e}^{(\bullet)}_n$ for matrix valued functions $\mathbf{C} = \mathbf{C}(q)$. At first an error bound in terms of ε_n is given for the correction term (22).
Lemma 2: For $2 \le k \le 4$ the correction term (22) satisfies

$$h^2\mathbf{L}_k(\mathbf{v}(t_n), ..., \mathbf{v}(t_{n-k+1})) - h^2\mathbf{L}_k(\mathbf{v}_n, ..., \mathbf{v}_{n-k+1}) = \mathscr{O}(h)\sum_{i=1}^{k}\varepsilon_{n+1-i}.$$

Proof: The definition of $\mathbf{L}_k$ in (22) shows that $h^2\mathbf{L}_k$ satisfies a Lipschitz condition with a constant of size $\mathscr{O}(h)$ Therefore, the assertion is a direct consequence of the global error equation (31c). ■

The recursion for global errors $\mathbf{e}_n^{\boldsymbol{\Delta}\mathbf{q}}$ for $n \geq k-1$ follows directly from this lemma and from Theorem 1 by subtracting (23b) from (24a)

$$\sum_{i=1}^{k} \gamma_i \mathbf{e}_{n+1-i}^{\boldsymbol{\Delta}\mathbf{q}} = \mathbf{e}_{n+1}^{\mathbf{v}} + \mathcal{O}(h) \sum_{i=1}^{k} \varepsilon_{n+1-i} + \frac{\mathbf{l}_n^q}{h} = \mathcal{O}(1)\varepsilon_{n+1} + \mathcal{O}(h) \sum_{i=1}^{k} \varepsilon_{n+1-i} + \mathcal{O}(h^k). \tag{33}$$

Lemma 3: The global errors $\mathbf{e}_n^{\mathbf{v}}$ satisfy for $n \geq k-1$

$$\sum_{i=0}^{k} \alpha_i \mathbf{e}_{n+1-i}^{\mathbf{v}} = -h \mathbf{e}_{n+1}^{\mathbf{M}^{-1}\mathbf{B}^T\boldsymbol{\lambda}} + \mathcal{O}(h)\varepsilon_{n+1} + \mathcal{O}(h^{k+1}), \tag{34a}$$

$$\sum_{i=1}^{k} \gamma_i \frac{\mathbf{e}_{n+2-i}^{\mathbf{Bv}} - \mathbf{e}_{n+1-i}^{\mathbf{Bv}}}{h} = -\mathbf{e}_{n+1}^{\mathbf{S}\boldsymbol{\lambda}} + \mathcal{O}(1)\varepsilon_{n+1} + \mathcal{O}(h^k) \tag{34b}$$

with $\mathbf{S}(q) := [\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T](q)$.

Proof:

a) At first, (23c) is multiplied by $\mathbf{M}(q_{n+1})$ and subtracted from (24b) multiplied by $\mathbf{M}(q(t_{n+1}))$ exploiting $\mathbf{G}(q_{n+1}) = \mathbf{G}(q(t_{n+1})) + \mathcal{O}(1)\varepsilon_{n+1}$ and $\mathbf{G}(q(t_{n+1})) = \mathbf{G}(q(t_n)) + \mathcal{O}(h)$ for matrix valued functions $\mathbf{G}(q)$ and $\mathbf{g}(t_{n+1}, q_{n+1}, \mathbf{v}_{n+1}) = \mathbf{g}(t_{n+1}, q(t_{n+1}), \mathbf{v}(t_{n+1})) + \mathcal{O}(1)\varepsilon_{n+1}$. With the global error definitions (31c) and Theorem 1 equation (34a) is directly obtained.

b) Equation (34b) follows from (34a) by multiplying with $\mathbf{B}(q(t_n))$ from the left, dividing by h and rewriting the sum in terms of γ_i. Note, that $\mathbf{B}(q_n) = \mathbf{B}(q(t_n)) + \mathcal{O}(h)$ by the technical assumption (32). ■

Lemma 4: The global errors $\mathbf{e}_n^q$ satisfy for $n \geq k-1$

$$\mathbf{e}_{n+1}^q = \mathbf{e}_n^q + h\mathbf{e}_n^{\boldsymbol{\Delta}\mathbf{q}} + \mathcal{O}(h)(\varepsilon_{n+1} + \varepsilon_n), \tag{35a}$$

$$\sum_{i=0}^{k} \alpha_i \mathbf{e}_{n+1-i}^q = \mathcal{O}(h) \sum_{i=0}^{k} \varepsilon_{n+1-i} + \mathcal{O}(h^{k+1}). \tag{35b}$$

With $\boldsymbol{\Delta}_h \mathbf{e}_n^q := \dfrac{\mathbf{e}_{n+1}^q - \mathbf{e}_n^q}{h}$ we get for $n \geq k-1$

$$\sum_{i=1}^{k} \gamma_i \boldsymbol{\Delta}_h \mathbf{e}_{n+1-i}^q = \mathbf{e}_{n+1}^{\mathbf{v}} + \frac{\mathbf{l}_n^q}{h} + \sum_{i=1}^{k} \gamma_i \widehat{\mathbf{e}}_{n+1-i}^q \boldsymbol{\Delta}\mathbf{q}(t_n) + \mathcal{O}(h) \left(\sum_{i=0}^{k} \varepsilon_{n+1-i} + \sum_{i=1}^{k} \|\boldsymbol{\Delta}_h \mathbf{e}_{n+1-i}^q\| \right) \tag{36a}$$

where

$$\sum_{i=1}^{k} \gamma_i \boldsymbol{\Delta}_h \mathbf{e}_{n+1-i}^q = \mathcal{O}(1) \sum_{i=0}^{k} \varepsilon_{n+1-i} + \mathcal{O}(h) \sum_{i=1}^{k} \|\boldsymbol{\Delta}_h \mathbf{e}_{n+1-i}^q\| + \mathcal{O}(h^k). \tag{36b}$$

Proof: Inserting (23a) and (25) into (31a), formula

$$\begin{aligned} \exp(\widetilde{\mathbf{e}}_{n+1}^q) &= q_{n+1}^{-1} \circ q(t_{n+1}) \\ &= \exp(-h\widetilde{\boldsymbol{\Delta}\mathbf{q}}_n) \circ q_n^{-1} \circ q(t_n) \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)) \\ &= \exp(-h\widetilde{\boldsymbol{\Delta}\mathbf{q}}_n) \circ \exp(\widetilde{\mathbf{e}}_n^q) \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)) \\ &= \exp(-h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n) + h\widetilde{\mathbf{e}}_n^{\boldsymbol{\Delta}\mathbf{q}}) \circ \exp(\widetilde{\mathbf{e}}_n^q) \circ \exp(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)) \end{aligned} \tag{37}$$

is obtained [10]. This product is studied applying twice the Baker-Campbell-Hausdorff formula, see [11, Lemma III.4.3]:

$$\begin{aligned} \exp(\widetilde{\mathbf{e}}_{n+1}^q) &= \exp\left(-h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n) + h\widetilde{\mathbf{e}}_n^{\boldsymbol{\Delta}\mathbf{q}} + \widetilde{\mathbf{e}}_n^q - \frac{h}{2}[\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n), \widetilde{\mathbf{e}}_n^q] + \mathcal{O}(h^2)\varepsilon_n + \mathcal{O}(h^2)\|\mathbf{e}_n^{\boldsymbol{\Delta}\mathbf{q}}\| \right) \circ \exp\left(h\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n) \right) \\ &= \exp\left(\widetilde{\mathbf{e}}_n^q + h\widetilde{\mathbf{e}}_n^{\boldsymbol{\Delta}\mathbf{q}} - \frac{h}{2}[\widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n), \widetilde{\mathbf{e}}_n^q] + \frac{h}{2}[\widetilde{\mathbf{e}}_n^q, \widetilde{\boldsymbol{\Delta}\mathbf{q}}(t_n)] + \mathcal{O}(h^2)\varepsilon_n + \mathcal{O}(h^2)\|\mathbf{e}_n^{\boldsymbol{\Delta}\mathbf{q}}\| \right). \end{aligned}$$

By considering the argument of the exponential map, we get

$$\mathbf{e}^q_{n+1} = \mathbf{e}^q_n + h\mathbf{e}^{\mathbf{\Delta} q}_n + h\widehat{\mathbf{e}}^q_n \mathbf{\Delta q}(t_n) + \mathcal{O}(h^2)\varepsilon_n + \mathcal{O}(h^2)\|\mathbf{e}^{\mathbf{\Delta q}}_n\|, \tag{38}$$

and

$$(\mathbf{I} + \mathcal{O}(h))\mathbf{e}^{\mathbf{\Delta q}}_n = \mathbf{\Delta}_h \mathbf{e}^q_n + \mathcal{O}(1)\varepsilon_n, \tag{39}$$

i.e., $h\mathbf{e}^{\mathbf{\Delta q}}_n = \mathcal{O}(1)(\varepsilon_{n+1} + \varepsilon_n)$ and (35a) follows directly.
Looking at $\sum_{i=1}^k \gamma_i(\mathbf{e}^q_{n+2-i} - \mathbf{e}^q_{n+1-i})$ and by inserting (38), (39) and (33), equation

$$\begin{aligned}
\sum_{i=1}^k \gamma_i \mathbf{\Delta}_h \mathbf{e}^q_{n+1-i} &= \sum_{i=1}^k \gamma_i \frac{(\mathbf{e}^q_{n+2-i} - \mathbf{e}^q_{n+1-i})}{h} \\
&= \sum_{i=1}^k \gamma_i (\mathbf{e}^{\mathbf{\Delta q}}_{n+1-i} + \widehat{\mathbf{e}}^q_{n+1-i}\mathbf{\Delta q}(t_n) + \mathcal{O}(h)\varepsilon_{n+1-i} + \mathcal{O}(h)\|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\|) \\
&= \mathbf{e}^{\mathbf{v}}_{n+1} + \frac{\mathbf{l}^q_n}{h} + \sum_{i=1}^k \gamma_i \widehat{\mathbf{e}}^q_{n+1-i}\mathbf{\Delta q}(t_n) + \mathcal{O}(h)\sum_{i=0}^k \varepsilon_{n+1-i} + \mathcal{O}(h)\sum_{i=1}^k \|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\|
\end{aligned}$$

is obtained and therefore estimates (36a) and (36b). Rewriting this sum in terms of α_i, we get estimate (35b), since $h\|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\| \leq \varepsilon_{n+1-i} + \varepsilon_{n+2-i}$. ■

For constrained mechanical systems, the holonomic constraints (23d) must be taken into consideration. With the next lemma, an estimation of the products of the constraint matrix $\mathbf{B}(q)$ with error terms $\mathbf{e}^q_n$ is obtained, which is needed to get a global error bound for the Lagrange multipliers $\boldsymbol{\lambda}$. The proof of this lemma is given in detail in [10, Lemma 4] for the generalized-α method.

Lemma 5: Define $\varphi_n := \mathbf{\Phi}(q_n)$ with $\varphi_n = \mathbf{0}$ for $n > k-1$, see (23d). The global errors $\mathbf{e}^q_n$ satisfy for $2 \leq k \leq 4$ and $n \geq k-1$

$$\begin{aligned}
\mathbf{0} &= \mathbf{B}(q(t_n))\mathbf{e}^q_n + \varphi_n + \mathcal{O}(h)\varepsilon_n, && (40a) \\
\mathbf{B}(q(t_n))\sum_{i=1}^k \gamma_i \mathbf{\Delta}_h \mathbf{e}^q_{n+1-i} &= -\sum_{i=1}^k \gamma_i \mathbf{Z}(q(t_n))(\mathbf{e}^q_{n+1-i}, \mathbf{v}(t_n)) - \sum_{i=1}^k \gamma_i \frac{\varphi_{n+2-i} - \varphi_{n+1-i}}{h} \\
&\quad + \mathcal{O}(h)\left(\sum_{i=1}^k \varepsilon_{n+1-i} + \|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\|\right) && (40b)
\end{aligned}$$

with the bilinear form $\mathbf{Z}(q)$ from (19).

Proof:

a) Equation (40a) follows as in [10, Lemma 4] from (23d) and (17c), because of definition (18).

b) From [10, Lemma 4]

$$\mathbf{B}(q(t_n))\mathbf{\Delta}_h \mathbf{e}^q_n + \mathbf{Z}(q(t_n))(\mathbf{e}^q_n, \mathbf{v}(t_n)) = -\frac{\varphi_{n+1} - \varphi_n}{h} + \mathcal{O}(h)(\varepsilon_n + \|\mathbf{\Delta}_h \mathbf{e}^q_n\|)$$

is obtained. Looking at $\sum_{i=1}^k \gamma_i \left(\mathbf{B}(q(t_n))\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i} + \mathbf{Z}(q(t_n))(\mathbf{e}^q_{n+1-i}, \mathbf{v}(t_n))\right)$ the assertion follows with (32). ■

Lemma 6: For $n \geq 2k-1$, the global errors $\mathbf{e}^{\mathbf{Bv}}_n$ satisfy

$$\sum_{i=1}^k \gamma_i \frac{\mathbf{e}^{\mathbf{Bv}}_{n+2-i} - \mathbf{e}^{\mathbf{Bv}}_{n+1-i}}{h} = \mathcal{O}\left(\frac{1}{h^2}\right)\max_r \|\varphi_r\| + \mathcal{O}(1)\left(\sum_{i=0}^{2k} \varepsilon_{n+1-i} + \sum_{i=1}^{2k} \|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\|\right) + \mathcal{O}(h^k). \tag{41}$$

Proof: Inserting (36a) into (40b), it follows for $n \geq k-1$

$$\begin{aligned}\mathbf{e}^{\mathbf{Bv}}_{n+1} &= -\frac{\mathbf{B}(q(t_n))\mathbf{l}^q_n}{h} - \sum_{i=1}^{k} \gamma_i h \mathbf{r}_h(t_{n+1-i}, \mathbf{e}^q_{n+1-i}) - \sum_{i=1}^{k} \gamma_i \frac{\varphi_{n+2-i} - \varphi_{n+1-i}}{h} \\ &\quad + \mathscr{O}(h) \left(\sum_{i=0}^{k} \varepsilon_{n+1-i} + \sum_{i=1}^{k} \|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\| \right) \end{aligned} \tag{42}$$

with the vector valued function

$$\mathbf{r}_h(t_n, \mathbf{e}^q_n) := \frac{1}{h}\Big(\mathbf{Z}(q(t_n))(\mathbf{e}^q_n, \mathbf{v}(t_n)) + \mathbf{B}(q(t_n))\widehat{\mathbf{e}}^q_n \mathbf{\Delta q}(t_n)\Big) \tag{43}$$

that is linear in $\mathbf{e}^q_n$ and satisfies the estimate

$$\sum_{i=1}^{k} \gamma_i \left(\mathbf{r}_h(t_{n+2-i}, \mathbf{e}^q_{n+2-i}) - \mathbf{r}_h(t_{n+1-i}, \mathbf{e}^q_{n+1-i})\right) = \mathscr{O}(1) \left(\sum_{i=1}^{k} \varepsilon_{n+1-i} + \sum_{i=1}^{k} \|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\| \right). \tag{44}$$

Looking at $\sum_{i=1}^{k} \gamma_i \frac{\mathbf{e}^{\mathbf{Bv}}_{n+2-i} - \mathbf{e}^{\mathbf{Bv}}_{n+1-i}}{h}$ the assertion is obtained with (27) and (44).

■

Lemma 7: The global errors $\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_n$ satisfy for $n \geq 2k-1$

$$\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1} = \mathscr{O}\left(\frac{1}{h^2}\right) \max_r \|\varphi_r\| + \mathscr{O}(1) \left(\sum_{i=0}^{2k} \varepsilon_{n+1-i} + \sum_{i=1}^{2k} \|\mathbf{\Delta}_h \mathbf{e}^q_{n+1-i}\| \right) + \mathscr{O}(h^k). \tag{45}$$

Proof: The assertion is obtained by inserting (41) into (34b). ■

Note that this error depends on $2k$ past values. Therefore we will consider the case that there are $2k$ starting values in the next theorem. In Section 3.3 the starting phase will be examined to prove the convergence over the whole time interval.

Theorem 2: Let the order conditions (3) be fulfilled and suppose that the starting values $q_0, ..., q_{2k-1}$, $\mathbf{v}_0, ..., \mathbf{v}_{2k-1}$ and $\boldsymbol{\lambda}_0, ..., \boldsymbol{\lambda}_{2k-1}$ satisfy

$$\sum_{i=0}^{2k-1} \|\mathbf{e}^q_i\| = \mathscr{O}(h^{k+1}), \; \sum_{i=0}^{2k-1} \|\mathbf{e}^{\mathbf{v}}_i\| + \|\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_i\| = \mathscr{O}(h^k), \max_{0 \leq i \leq 2k-1} \|\varphi_i\| = \mathscr{O}(h^{k+2}). \tag{46}$$

Then, there are positive constants $\widetilde{C}$, $\widetilde{L}$ and h_0 independent of n and h, such that for all $h \in (0, h_0]$ and all $n \geq 0$ with $t_0 + nh \leq t_{\text{end}} - h$ the following global error bounds hold

$$\|\mathbf{e}^q_n\| + \|\mathbf{e}^{\mathbf{v}}_n\| + \|\mathbf{e}^{\boldsymbol{\lambda}}_n\| \leq \widetilde{C} e^{\widetilde{L}(t_n - t_0)} h^k. \tag{47}$$

Proof: For $0 \leq n < 2k-1$ the assertion follows directly from the assumption (46). For $n \geq 2k-1$ a one-step error recursion for the k-step BLieDF2$^{\text{nd}}$ method (23) can be obtained by combining the estimates (35b), (34a), (36b) and (45) for $n \geq 2k-1$ to

$$\begin{aligned} \|\mathbf{E}^{\mathbf{y}}_{n+1} - \mathbf{T}_{\mathbf{y}} \mathbf{E}^{\mathbf{y}}_n\| &\leq \mathscr{O}(h)(\|\mathbf{E}^{\mathbf{y}}_{n+1}\| + \|\mathbf{E}^{\mathbf{z}}_{n+1}\|) + \mathscr{O}(h^{k+1}) \\ \|\mathbf{E}^{\mathbf{z}}_{n+1} - \mathbf{T}_{\mathbf{z}} \mathbf{E}^{\mathbf{z}}_n\| &\leq \mathscr{O}(1)(\|\mathbf{E}^{\mathbf{y}}_{n+1}\| + \|\mathbf{E}^{\mathbf{y}}_n\| + h\|\mathbf{E}^{\mathbf{z}}_{n+1}\| + h\|\mathbf{E}^{\mathbf{z}}_n\|) + \mathscr{O}(h^k) \end{aligned}$$

with

$$\mathbf{E}^{\mathbf{y}}_n := \begin{bmatrix} \mathbf{e}^q_n \\ \vdots \\ \mathbf{e}^q_{n+1-2k} \\ \mathbf{e}^{\mathbf{v}}_n \\ \vdots \\ \mathbf{e}^{\mathbf{v}}_{n+1-2k} \end{bmatrix}, \; \mathbf{E}^{\mathbf{z}}_n = \begin{bmatrix} \mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_n \\ \vdots \\ \mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1-2k} \\ \mathbf{\Delta}_h \mathbf{e}^q_{n-1} \\ \vdots \\ \mathbf{\Delta}_h \mathbf{e}^q_{n+1-2k} \end{bmatrix}, \; \mathbf{T}_q := \begin{bmatrix} -\frac{\alpha_1}{\alpha_0} & -\frac{\alpha_2}{\alpha_0} & \cdots & -\frac{\alpha_k}{\alpha_0} \\ 1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \vdots \\ & & 1 & 0 \\ & & & 1 \end{bmatrix}, \; \mathbf{T}_{\mathbf{\Delta q}} = \begin{bmatrix} -\frac{\gamma_2}{\gamma_1} & -\frac{\gamma_3}{\gamma_1} & \cdots & -\frac{\gamma_k}{\gamma_1} \\ 1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \vdots \\ & & 1 & 0 \\ & & & 1 \end{bmatrix} \tag{48a}$$

and

$$\mathbf{J}=\begin{bmatrix}0 & \cdots & & 0\\ 1 & 0 & \cdots & 0\\ & \ddots & \ddots & \vdots\\ 0 & & 1 & 0\end{bmatrix}\in\mathbb{R}^{k\times k},\ \mathbf{T_y}:=\begin{bmatrix}\mathbf{T}_q & \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k}\\ \mathbf{0}_{k\times k} & \mathbf{J} & \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k}\\ \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k} & \mathbf{T}_q & \mathbf{0}_{k\times k}\\ \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k} & \mathbf{0}_{k\times k} & \mathbf{J}\end{bmatrix}\otimes\mathbf{I},\ \mathbf{T_z}:=\begin{bmatrix}\mathbf{J} & \mathscr{O}(1)\\ \mathbf{0}_{k-1,k} & \mathbf{T_{\Delta q}}\end{bmatrix}\otimes\mathbf{I}. \tag{48b}$$

The term $\frac{1}{h^2}\max_r\|\varphi_r\|$ in (45) is $\mathscr{O}(h^k)$, because of (46) and $\varphi_r=\mathbf{0}$ for $r\geq k$.
Therefore, a positive constant L independent of h and n and an appropriate constant $M\geq 0$, that represents the local error terms $\mathscr{O}(h^k)$, can be found, such that for $n\geq 2k-1$

$$\|\mathbf{E}^{\mathbf{y}}_{n+1}-\mathbf{T_y}\mathbf{E}^{\mathbf{y}}_{n}\| \leq Lh(\|\mathbf{E}^{\mathbf{y}}_{n+1}\|+\|\mathbf{E}^{\mathbf{z}}_{n+1}\|)+hM, \tag{49a}$$
$$\|\mathbf{E}^{\mathbf{z}}_{n+1}-\mathbf{T_z}\mathbf{E}^{\mathbf{z}}_{n}\| \leq L(\|\mathbf{E}^{\mathbf{y}}_{n+1}\|+\|\mathbf{E}^{\mathbf{y}}_{n}\|+h\|\mathbf{E}^{\mathbf{z}}_{n+1}\|+h\|\mathbf{E}^{\mathbf{z}}_{n}\|)+M. \tag{49b}$$

From [9, Lemma III.4.4] it is known that there is a norm $\|.\|_q$ with $\|\mathbf{T_y}\|_q=1$. Since the spectral radius yields $\rho(\mathbf{J})=0$, a norm $\|.\|_\varepsilon$ for every $\varepsilon>0$ exists with

$$\|\mathbf{J}\|_\varepsilon<\varepsilon. \tag{50}$$

The characteristic polynomial $p(\zeta)=\sum_{i=1}^k\gamma_i\zeta^{k-i}$ of matrix $\mathbf{T_{\Delta q}}$ has the same roots as $(\zeta-1)\sum_{i=1}^k\gamma_i\zeta^{k-i}=\sum_{i=0}^k\alpha_i\zeta^{k-i}$ except for the root $\zeta_1=1$. The other roots satisfy $|\zeta_i|<1$, see [9]. For that reason there exists a norm with $\|\mathbf{T_{\Delta q}}\|<1$ and consequently with (50) a norm $\|.\|_{\mathbf{z}}$ with $\|\mathbf{T_z}\|_{\mathbf{z}}<1$.
With [3, Theorem 4.16] the estimates for step sizes $h\in(0,h_0]$

$$\|\mathbf{E}^{\mathbf{y}}_{n}\| \leq e^{\overline{L}(t_n-t_0)}(\|\mathbf{E}^{\mathbf{y}}_{2k-1}\|+\overline{C}h\|\mathbf{E}^{\mathbf{z}}_{2k-1}\|)+\frac{e^{\overline{L}(t_n-t_0)}-1}{L}\overline{M}, \tag{51a}$$
$$\|\mathbf{E}^{\mathbf{z}}_{n+1}-\mathbf{T}_{\mathbf{z}}^{n+1-2k}\mathbf{E}^{\mathbf{z}}_{2k-1}\| \leq \overline{C}e^{\overline{L}(t_n-t_0)}(\|\mathbf{E}^{\mathbf{y}}_{2k-1}\|+h\|\mathbf{E}^{\mathbf{z}}_{2k-1}\|+\overline{M}) \tag{51b}$$

are obtained with $t_n:=t_0+nh$, $(n\geq 2k-1)$ and positive constants h_0, $\overline{C}$, $\overline{L}$, $\overline{M}$, that depends on the constants L and M, as well as on the chosen norms.
From (46), we know that $\|\mathbf{E}^{\mathbf{y}}_{2k-1}\|=\mathscr{O}(h^k)$ and $\|\mathbf{E}^{\mathbf{z}}_{2k-1}\|=\mathscr{O}(h^k)$. The assertion follows for $n\geq 2k-1$ by (51).■
With this theorem the convergence of the BLieDF2$^{\text{nd}}$ integrator is shown for $2\leq k\leq 4$ for all variables, if the conditions (46) are fulfilled. In the next section we want to take a closer look at the transient phase to prove the convergence also for $k-1<n<2k$. We will see that there is an order reduction in $\boldsymbol{\lambda}$ in this transient phase if the analytical solution is used for defining the starting values.

3.3 Starting phase and order reduction

Equation (45) is valid only for $n\geq 2k-1$. Therefore another estimate of the global error of $\boldsymbol{\lambda}$ is needed to prove the convergence in the starting phase.
Lemma 8: Let us suppose that the starting values $q_0,...,q_{k-1}$ and $\mathbf{v}_0,...,\mathbf{v}_{k-1}$ satisfy

$$\|\mathbf{e}^q_j\|=\mathscr{O}(h^{k+1}),\ \|\mathbf{e}^{\mathbf{Bv}}_j+\mathbf{B}(q(t_{k-1}))\frac{\mathbf{l}^q_{k-1}}{h}\|=\mathscr{O}(h^{k+1}),\ \|\varphi_j\|=\mathscr{O}(h^{k+2}) \tag{52}$$

for $j=0,...,k-1$, then the global errors $\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1}$ satisfy for $n=k-1,...,2k-1$

$$\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1}=\mathscr{O}(1)\left(\sum_{i=0}^{n+1}\varepsilon_{n+1-i}+\sum_{i=1}^{n+1}\|\boldsymbol{\Delta}_h\mathbf{e}^q_{n+1-i}\|\right)+\mathscr{O}(h^k). \tag{53}$$

Proof: Equation (34b) can be rewritten for $2k-1 \geq n \geq k-1$ to

$$\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1} = -\sum_{i=1}^{k} \gamma_i \frac{\left(\mathbf{e}^{\mathbf{Bv}}_{n+2-i} + \mathbf{B}(q(t_{n+1-i}))\frac{\mathbf{l}^q_{n+1-i}}{h}\right) - \left(\mathbf{e}^{\mathbf{Bv}}_{n+1-i} + \mathbf{B}(q(t_{n+1-i}))\frac{\mathbf{l}^q_{n+1-i}}{h}\right)}{h} + \mathscr{O}(1)\varepsilon_{n+1} + \mathscr{O}(h^k).$$

For $1 \leq i \leq n+2-k$ the difference can be examined by using equation (27), (42), (44) and assumption (52):

$$\begin{aligned}
&\frac{\left(\mathbf{e}^{\mathbf{Bv}}_{n+2-i} + \mathbf{B}(q(t_{n+1-i}))\frac{\mathbf{l}^q_{n+1-i}}{h}\right) - \left(\mathbf{e}^{\mathbf{Bv}}_{n+1-i} + \mathbf{B}(q(t_{n+1-i}))\frac{\mathbf{l}^q_{n+1-i}}{h}\right)}{h} \\
&= -\mathbf{B}(q(t_n))\frac{\mathbf{l}^q_{n+1-i} - \mathbf{l}^q_{n-i}}{h^2} - \sum_{j=1}^{k} \gamma_i (\mathbf{r}_h(t_{n+2-i-j}, \mathbf{e}^q_{n+2-i-j}) - \mathbf{r}_h(t_{n+1-i-j}, \mathbf{e}^q_{n+1-i-j})) \\
&\quad + \mathscr{O}\left(\frac{1}{h^2}\right)\max_r \|\boldsymbol{\varphi}_r\| + \mathscr{O}(1)\left(\sum_{j=0}^{k+1} \varepsilon_{n+2-i-j} + \sum_{j=1}^{k+1} \|\boldsymbol{\Delta}_h \mathbf{e}^q_{n+2-i-j}\|\right) + \mathscr{O}(h^k) \\
&= \mathscr{O}(1)\left(\sum_{j=0}^{k+1} \varepsilon_{n+2-i-j} + \sum_{j=1}^{k+1} \|\boldsymbol{\Delta}_h \mathbf{e}^q_{n+2-i-j}\|\right) + \mathscr{O}(h^k).
\end{aligned}$$

For $n+3-k \leq i \leq k$ this difference is treated by using the assumption (52):

$$\frac{\left(\mathbf{e}^{\mathbf{Bv}}_{n+2-i} + \mathbf{B}(q(t_{n+1-i}))\frac{\mathbf{l}^q_{n+1-i}}{h}\right) - \left(\mathbf{e}^{\mathbf{Bv}}_{n+1-i} + \mathbf{B}(q(t_{n+1-i}))\frac{\mathbf{l}^q_{n+1-i}}{h}\right)}{h} = \mathscr{O}(h^k).$$

All in all we get

$$\begin{aligned}
\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1} &= \mathscr{O}(1)\sum_{i=1}^{n+1-k}\left(\sum_{j=0}^{k+1} \varepsilon_{n+2-i-j} + \sum_{j=1}^{k+1} \|\boldsymbol{\Delta}_h \mathbf{e}^q_{n+2-i-j}\|\right) + \mathscr{O}(1)\varepsilon_{n+1} + \mathscr{O}(h^k) \\
&= \mathscr{O}(1)\left(\sum_{i=0}^{n+1} \varepsilon_{n+1-i} + \sum_{i=1}^{n+1} \|\boldsymbol{\Delta}_h \mathbf{e}^q_{n+1-i}\|\right) + \mathscr{O}(h^k).
\end{aligned}$$

■

Theorem 3: Let the order conditions (3) be fulfilled and suppose that the starting values $q_0, \ldots, q_{k-1}$, $\mathbf{v}_0, \ldots, \mathbf{v}_{k-1}$ and $\boldsymbol{\lambda}_0, \ldots, \boldsymbol{\lambda}_{k-1}$ satisfy (52) and

$$\|\mathbf{e}^{\mathbf{v}}_j\| + \|\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_j\| = \mathscr{O}(h^k) \tag{54}$$

for $j = 0, \ldots, k-1$. Then, there are positive constants $\overline{C}$, $\overline{L}$ and h_0 independent of n and h, such that for all $h \in (0, h_0]$ and all $0 \leq n \leq 2k-1$ with $t_0 + nh \leq t_{\text{end}} - h$ the following global error bounds hold

$$\|\mathbf{e}^q_n\| \leq \overline{C}e^{\overline{L}(t_n - t_0)}h^{k+1}, \ \|\mathbf{e}^{\mathbf{v}}_n\| + \|\mathbf{e}^{\boldsymbol{\lambda}}_n\| \leq \overline{C}e^{\overline{L}(t_n - t_0)}h^k. \tag{55}$$

Proof: We want to prove this by induction. For $0 \leq n \leq k-1$ estimate (55) is valid, because of assumptions (54). Let the assertion be fulfilled for all $i \leq n$ and show that its also valid for $n+1 \leq 2k-1$. By using this induction assertion equations (34a), (35b), (36b) and (53) can be rewritten for $k-1 \leq n < 2k-1$ to

$$\begin{aligned}
\mathbf{e}^q_{n+1} &= \mathscr{O}(h)\varepsilon_{n+1} - \sum_{i=1}^{k}\frac{\alpha_i}{\alpha_0}\mathbf{e}^q_{n+1-i} + \mathscr{O}(h)\sum_{i=1}^{k}\varepsilon_{n+1-i} + \mathscr{O}(h^{k+1}) = \mathscr{O}(h)\varepsilon_{n+1} + \mathscr{O}(h^{k+1}), \\
\mathbf{e}^{\mathbf{v}}_{n+1} &= -\frac{h}{\alpha_0}\mathbf{e}^{\mathbf{M}^{-1}\mathbf{B}\boldsymbol{\lambda}}_{n+1} + \mathscr{O}(h)\varepsilon_{n+1} - \sum_{i=1}^{k}\frac{\alpha_i}{\alpha_0}\mathbf{e}^{\mathbf{v}}_{n+1-i} + \mathscr{O}(h^{k+1}) = -\frac{h}{\alpha_0}\mathbf{e}^{\mathbf{M}^{-1}\mathbf{B}\boldsymbol{\lambda}}_{n+1} + \mathscr{O}(h)\varepsilon_{n+1} + \mathscr{O}(h^k), \\
\mathbf{e}^{\mathbf{S}\boldsymbol{\lambda}}_{n+1} &= \mathscr{O}(1)(\varepsilon_{n+1} + \|\boldsymbol{\Delta}_h \mathbf{e}^q_n\|) + \mathscr{O}(1)\left(\sum_{i=1}^{n+1}\varepsilon_{n+1-i} + \sum_{i=2}^{n+1}\|\boldsymbol{\Delta}_h \mathbf{e}^q_{n+1-i}\|\right) + \mathscr{O}(h^k) \\
&= \mathscr{O}(1)(\varepsilon_{n+1} + \|\boldsymbol{\Delta}_h \mathbf{e}^q_n\|) + \mathscr{O}(h^k)
\end{aligned}$$

and

$$\begin{aligned}\mathbf{\Delta}_h\mathbf{e}_n^q &= \mathscr{O}(1)\varepsilon_{n+1}+\mathscr{O}(h)\|\mathbf{\Delta}_h\mathbf{e}_n^q\|-\sum_{i=2}^{k}\frac{\gamma_i}{\gamma_1}\mathbf{\Delta}_h\mathbf{e}_{n+1-i}^q+\mathscr{O}(1)\sum_{i=1}^{k}\varepsilon_{n+1-i}+\mathscr{O}(h)\sum_{i=2}^{k}\|\mathbf{\Delta}_h\mathbf{e}_{n+1-i}^q\|+\mathscr{O}(h^k)\\ &= \mathscr{O}(1)\varepsilon_{n+1}+\mathscr{O}(h)\|\mathbf{\Delta}_h\mathbf{e}_n^q\|+\mathscr{O}(h^k).\end{aligned}$$

Therefore we get

$$\begin{aligned}(1+\mathscr{O}(h))\|\mathbf{e}_{n+1}^q\| &= \mathscr{O}(h)\|\mathbf{e}_{n+1}^{\mathbf{v}}\|+\mathscr{O}(h^2)\|\mathbf{e}_{n+1}^{\mathbf{S}\boldsymbol{\lambda}}\|+\mathscr{O}(h^{k+1}),\\ (1+\mathscr{O}(h))\|\mathbf{e}_{n+1}^{\mathbf{v}}\| &= \mathscr{O}(h)\|\mathbf{e}_{n+1}^q\|+\mathscr{O}(h)\|\mathbf{e}_{n+1}^{\mathbf{S}\boldsymbol{\lambda}}\|+\mathscr{O}(h^k),\\ (1+\mathscr{O}(h))\|\mathbf{e}_{n+1}^{\mathbf{S}\boldsymbol{\lambda}}\| &= \mathscr{O}(1)\|\mathbf{e}_{n+1}^q\|+\mathscr{O}(1)\|\mathbf{e}_{n+1}^{\mathbf{v}}\|+\mathscr{O}(1)\|\mathbf{\Delta}_h\mathbf{e}_{n+1}^q\|+\mathscr{O}(h^k),\\ (1+\mathscr{O}(h))\|\mathbf{\Delta}_h\mathbf{e}_{n+1}^q\| &= \mathscr{O}(1)\|\mathbf{e}_{n+1}^q\|+\mathscr{O}(1)\|\mathbf{e}_{n+1}^{\mathbf{v}}\|+\mathscr{O}(h)\|\mathbf{e}_{n+1}^{\mathbf{S}\boldsymbol{\lambda}}\|+\mathscr{O}(h^k)\end{aligned}$$

and estimates (55) follow by solving this equation system. ■

All in all the convergence of the BLieDF2[nd] integrator is proved over the whole time interval in the index-3 formulation, if Theorems 2 and 3 are combined. Note, that estimates (55) in the transient phase can only be guaranteed if $\|\mathbf{e}_j^{\mathbf{Bv}}+\mathbf{B}(q(t_{k-1}))\frac{\mathbf{l}_{k-1}^q}{h}\|=\mathscr{O}(h^{k+1})$ for $j=0,...,k-1$, see (52), otherwise equation (53) does not hold and there is an order reduction in $\boldsymbol{\lambda}$. If the analytical solutions $\mathbf{v}(t_j)$ are used as starting value $\mathbf{v}_j$ for $j=0,...,k-1$, the relationship

$$\|\mathbf{e}_j^{\mathbf{Bv}}+\mathbf{B}(q(t_{k-1}))\frac{\mathbf{l}_{k-1}^q}{h}\|=\|\mathbf{v}(t_j)-\mathbf{v}_j+\mathbf{B}(q(t_{k-1}))\frac{\mathbf{l}_{k-1}^q}{h}\|=\|\mathbf{B}(q(t_{k-1}))\frac{\mathbf{l}_{k-1}^q}{h}\|=\mathscr{O}(h^k)$$

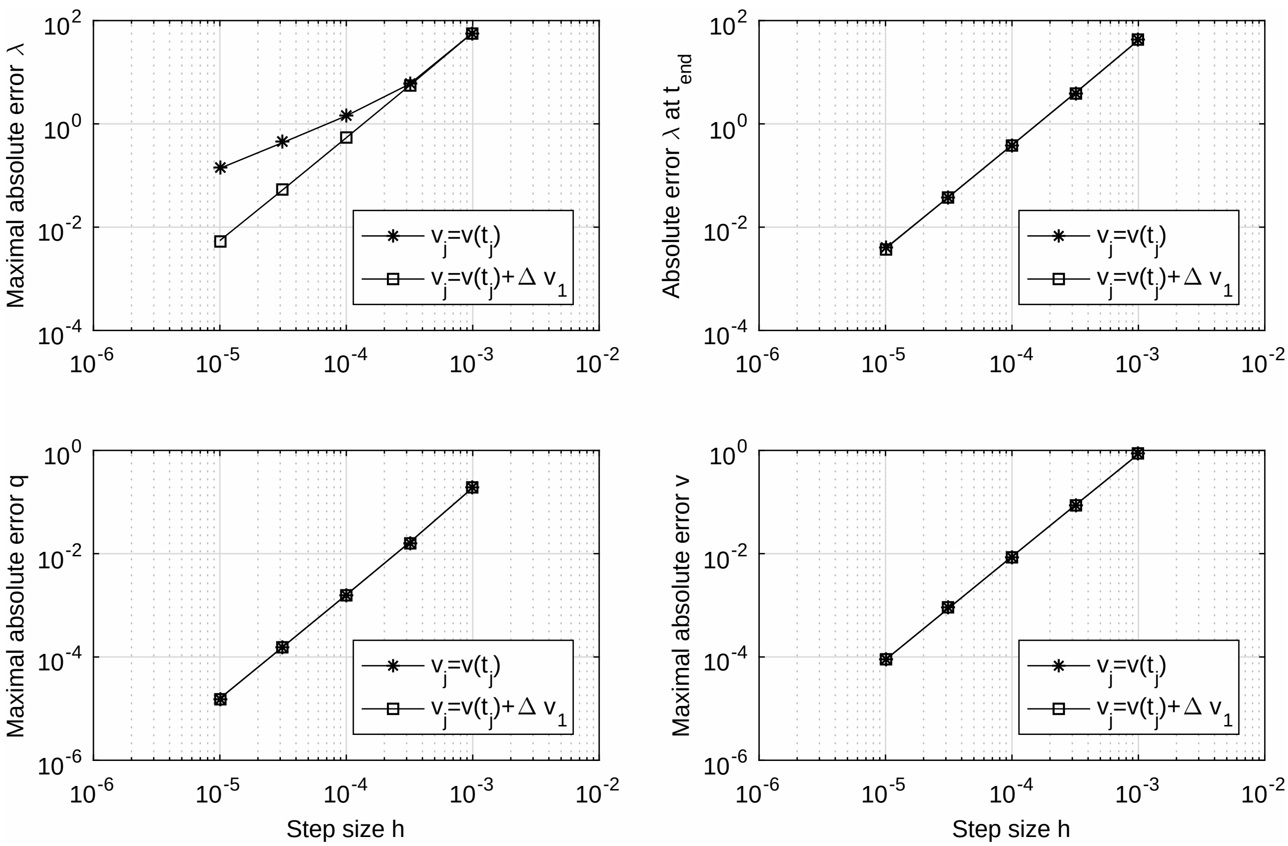

Fig. 1: Global errors for $k=2$ for the Heavy top benchmark with and without modification of $\mathbf{v}_0$ and $\mathbf{v}_1$ (Upper left plot: Lagrange multipliers $\boldsymbol{\lambda}$ - maximal absolute error in $[t_0,t_{\text{end}}]$. Upper right plot: Lagrange multipliers $\boldsymbol{\lambda}$ - absolute error at t_{end}. Lower left plot: position coordinate q - maximal absolute error in $[t_0,t_{\text{end}}]$. Lower right plot: velocity coordinate $\mathbf{v}$- maximal absolute error in $[t_0,t_{\text{end}}]$.)

follows with Theorem 1 and (52) can not be guaranteed generally. Therefore a modification of the k starting values $\mathbf{v}_j$ for $j = 0, \ldots, k-1$ is needed to avoid this order reduction in $\boldsymbol{\lambda}$. This modification can be chosen as

$$\mathbf{v}_j = \mathbf{v}(t_j) + \boldsymbol{\Delta}\mathbf{v}_{k-1}, \tag{56}$$

where $\boldsymbol{\Delta}\mathbf{v}_{k-1}$ can be computed by solving the system

$$\begin{bmatrix} \mathbf{M}(q(t_{k-1})) & \mathbf{B}^T(q(t_{k-1})) \\ \mathbf{B}(q(t_{k-1})) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Delta}\mathbf{v}_{k-1} \\ \boldsymbol{\Delta}\boldsymbol{\lambda}_{k-1} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{B}(q(t_{k-1}))\frac{\overline{\mathbf{l}^q_{k-1}}}{h} \end{bmatrix}$$

with the auxiliary vector $\boldsymbol{\Delta}\boldsymbol{\lambda}_{k-1}$, that is not needed in the following and an approximation $\overline{\mathbf{l}^q_{k-1}}$ of the leading local error term satisfying

$$\overline{\mathbf{l}^q_{k-1}} \;=\; \mathbf{l}^q_{k-1} + \mathscr{O}(h^{k+2}).$$

Furthermore approximations of the derivatives of $\mathbf{v}(t)$ at $t = t_k$ are needed in the evaluation of $\overline{\mathbf{l}^q_{k-1}}$, see Theorem 1. For $k = 2$ this would be $\dot{\mathbf{v}}_1 = \dot{\mathbf{v}}(t_1) + \mathscr{O}(h)$ and $\ddot{\mathbf{v}}_1 = \ddot{\mathbf{v}}(t_1) + \mathscr{O}(h)$.
In Figure 1 the order reduction of $\boldsymbol{\lambda}$ in the transient phase is shown for $k = 2$ for the Heavy top benchmark in the Lie group formulation $\mathbb{R}^3 \times SO(3)$ (see Section 4). For $\mathbf{v}_1 = \mathbf{v}(t_1)$ the maximal absolute error of $\boldsymbol{\lambda}$ decreases to order one. After the transient phase the expected global errors of size $\mathscr{O}(h^2)$ can be observed. In the other variables and if the starting values $\mathbf{v}_0$ and $\mathbf{v}_1$ are adapted as in (56), the global errors are of second order over the whole time interval.

4 Numerical results

4.1 Benchmark: Heavy top

To verify the theoretical results numerically, the benchmark problem Heavy top, see [13], is used. The Heavy top is a rotating, spinning top with its tip being fixed at the origin. The equations of motion for the unconstrained system in the Lie group formulation $SO(3)$ are given by (see [1]),

$$\dot{\mathbf{R}} \;=\; \mathbf{R}\widetilde{\boldsymbol{\Omega}}, \tag{57a}$$
$$\mathbf{0} \;=\; \mathbf{J}\dot{\boldsymbol{\Omega}} + \widetilde{\boldsymbol{\Omega}}\mathbf{J}\boldsymbol{\Omega} - \widetilde{\mathbf{X}}\mathbf{R}^T m\boldsymbol{\gamma} \tag{57b}$$

with rotation matrix $\mathbf{R} \in SO(3)$, angular velocity $\boldsymbol{\Omega}$, inertia tensor $\mathbf{J} = \mathrm{diag}(15.234375, 0.46875, 15.234375)$ kg·m^2 with respect to the fixed point, reference point $\mathbf{X} = [0\ 1\ 0]^T$, mass $m = 15$ kg and acceleration vector of the gravitation field $\boldsymbol{\gamma} = [0\ 0\ -9.81]^T$ m/s^2. As initial conditions $\mathbf{R}(0) = \mathbf{I}_3$ and $\boldsymbol{\Omega}(0) = [0\ 150\ -4.61538]^T$ rad/s are chosen. $\dot{\mathbf{R}}(0)$ and $\dot{\boldsymbol{\Omega}}(0)$ are calculated fitting to the equations of motion (57).
The equations of motion in the index-3 formulation for the Lie group formulation $\mathbb{R}^3 \times SO(3)$ are given by (58), see [13]

$$\dot{\mathbf{x}} \;=\; \mathbf{u}, \tag{58a}$$
$$\dot{\mathbf{R}} \;=\; \mathbf{R}\widetilde{\boldsymbol{\Omega}}, \tag{58b}$$
$$\mathbf{0}_{3\times 1} \;=\; m\dot{\mathbf{u}} - m\boldsymbol{\gamma} - \mathbf{R}\boldsymbol{\lambda}, \tag{58c}$$
$$\mathbf{0}_{3\times 1} \;=\; \mathbf{J}\dot{\boldsymbol{\Omega}} + \widetilde{\boldsymbol{\Omega}}\mathbf{J}\boldsymbol{\Omega} + \widetilde{\mathbf{X}}\boldsymbol{\lambda}, \tag{58d}$$
$$\mathbf{0}_{3\times 1} \;=\; -\mathbf{R}^T\mathbf{x} + \mathbf{X}. \tag{58e}$$

In the numerical tests, the mass of the body $m = 15$ kg, tensor of inertia with respect to the centre of mass in the body-attached frame $\mathbf{J} = \mathrm{diag}(0.234375, 0.46875, 0.234375)$ kg·m^2, position of the centre of mass $\mathbf{X} = [0\ 1\ 0]^T$ and acceleration of gravity $\boldsymbol{\gamma} = [0\ 0\ -9.81]^T$ m/s^2 are used. Again the initial values are $\mathbf{R}(0) = \mathbf{I}_3$ and $\boldsymbol{\Omega}(0) = [0\ 150\ -4.61538]^T$ rad/s and the others are calculated according to constraint (58e) and its hidden counterpart at the level of velocity coordinates.

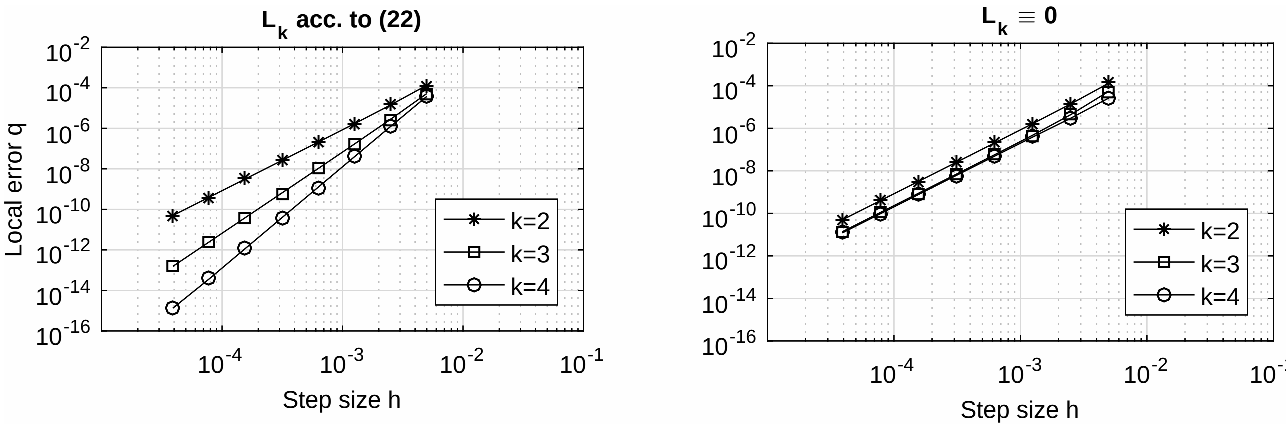

Fig. 2: Constrained system - local errors for the Heavy top benchmark (position coordinate q). Left plots: $\mathbf{L}_k$ according to (22). Right plots: $\mathbf{L}_k \equiv \mathbf{0}$.

4.2 Results

The numerical results are given for the example without kinematic constraints (57) in the Lie group formulation $SO(3)$ and for the example with kinematic constraints (58) in the Lie group formulation $\mathbb{R}^3 \times SO(3)$ for the Heavy top benchmark. For the test, a reference solution was calculated using the Matlab integrator ode15s with tight tolerances.

At first, the local errors are verified. The reference solution was used for the k starting values and one step of the BLieDF2$^{\text{nd}}$ integrator was done. Then the results were compared to the given reference solution and the absolute error of this result is given in Figure 2 for the variables q. The right plot shows the results with $\mathbf{L}_k \equiv \mathbf{0}$ for $2 \leq k \leq 4$ and the left one with $\mathbf{L}_k$ according to (22). It can be seen, that without this correction term $\mathbf{L}_k$, there is only a local error of order $\mathscr{O}(h^3)$ for $2 \leq k \leq 4$. If the definition (22) is used, then the local error decreases to order $\mathscr{O}(h^{k+1})$ as shown in Theorem 1.

Furthermore, the order of convergence was tested. In Figures 3 the reference solution is compared to the numerical solution for the unconstrained case with (left plots) and without (right plots) the correction term (22). The Heavy top benchmark was used until a time run up to $t_{\text{end}} = 2s$ and the relative global error at this time is given in Figure 3. As supposed, the numerical tests confirm global errors of size $\mathscr{O}(h^k)$ for $2 \leq k \leq 4$ for unconstrained mechanical systems when using the correction term (22). When $\mathbf{L}_k \equiv \mathbf{0}$ is used, we see that the convergence order decreases to $p = \min(2, k)$.

In Figure 4, the same numerical test was done for constrained mechanical systems in the index-3 formulation for the Heavy top benchmark. The reference solution is compared to the numerical solution for the position coordinates q (upper plots) and Lagrange multipliers $\boldsymbol{\lambda}$ (lower plots) with (left plots) and without (right plots) the correction

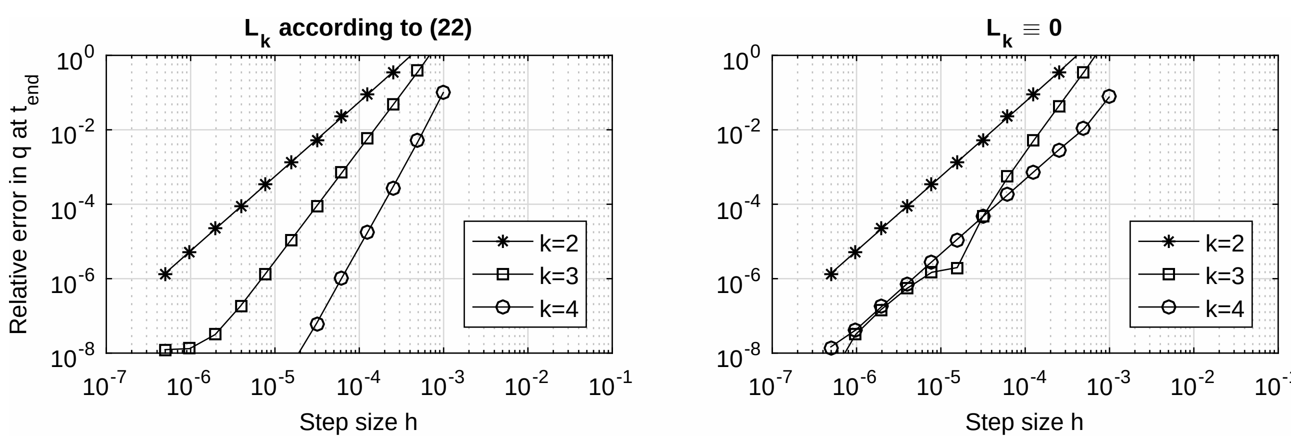

Fig. 3: Unconstrained system - global relative errors in q at $t_{\text{end}} = 2\text{s}$ for the Heavy top benchmark. Left plots: $\mathbf{L}_k$ according to (22). Right plots: $\mathbf{L}_k \equiv \mathbf{0}$

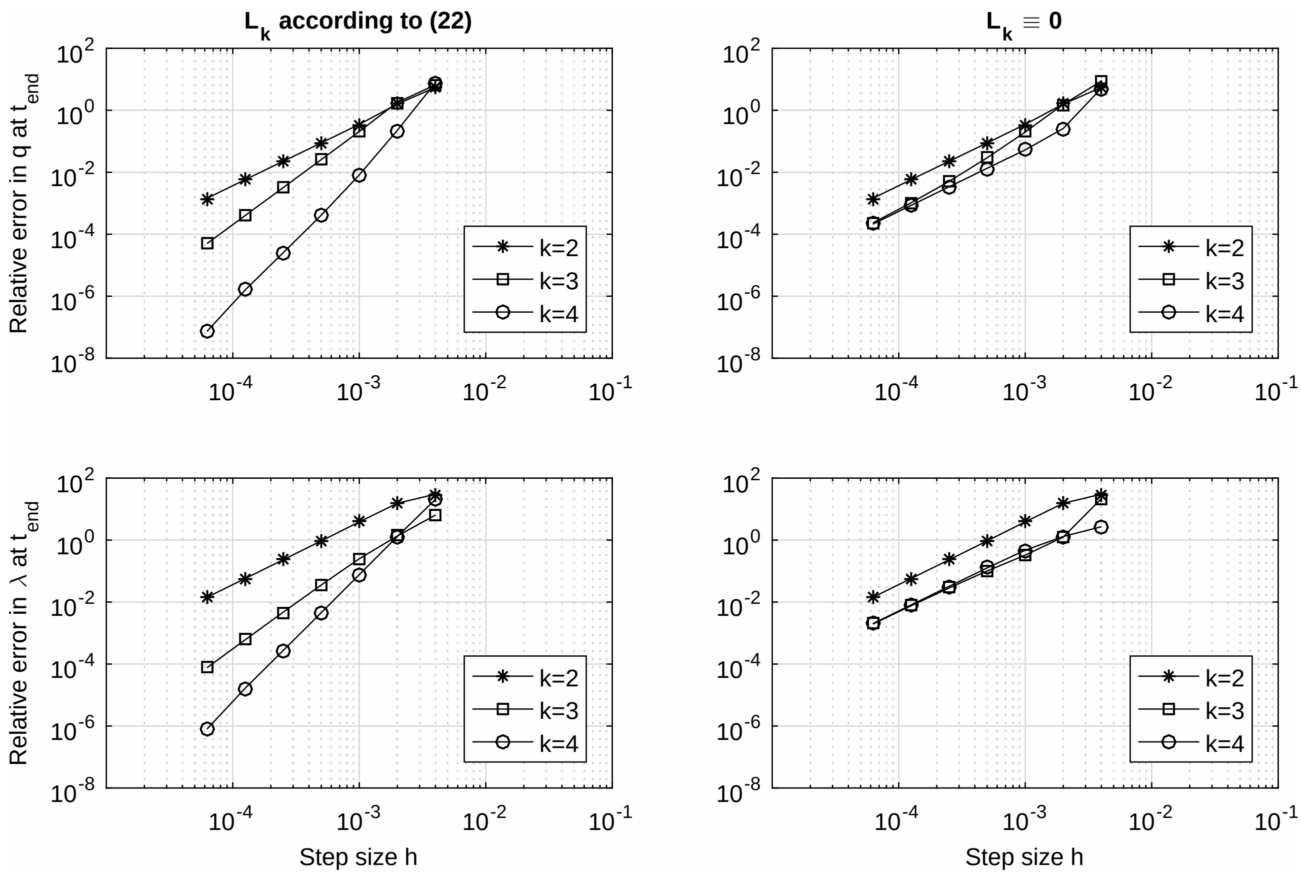

Fig. 4: Constrained system - global relative errors at $t_{\text{end}} = 2$s for the Heavy top benchmark. Left plots: $\mathbf{L}_k$ according to (22) (Upper plots: position coordinates q. Lower plots: Lagrange multipliers $\boldsymbol{\lambda}$) Right plots: $\mathbf{L}_k \equiv \mathbf{0}$ (Upper plots: position coordinates q. Lower plots: Lagrange multipliers $\boldsymbol{\lambda}$)

term (22). As for the unconstrained system, the numerical tests confirm the analytical proof of global errors of size $\mathscr{O}(h^k)$ for $2 \leq k \leq 4$ when using the correction term (22) and the convergence order $p = \min(2,k)$ when $\mathbf{L}_k \equiv \mathbf{0}$ is used. Therefore, we could confirm our theoretical studies numerically and saw that for $2 \leq k \leq 4$ only one commutator is needed to get the same order as in linear spaces.

5 Conclusions

All in all, the k-step BLieDF2$^{\text{nd}}$, a multistep method for unconstrained and constrained mechanical systems in Lie group formulation, was introduced in this paper. We could prove a local truncation error of size $\mathscr{O}(h^{k+1})$ and convergence order $p = k$ for $k = 2,3,4$, corresponding to the BDF methods for ODEs in linear spaces. For constrained systems, we observed an order reduction of $\boldsymbol{\lambda}$ in the transient phase if the analytical solution is used as starting value for the velocity coordinates. The results could be confirmed numerically for the Heavy top benchmark in the unconstrained Lie group formulation $SO(3)$ and in the constrained formulation in $\mathbb{R}^3 \times SO(3)$. In future research we want to prove convergence for the stabilized index-2 formulation and examine the BLieDF2$^{\text{nd}}$ integrator for $k = 5,6$.

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