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

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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 multi-step methods of BDF type which are the methods-of-choice in most industrial multibody system simulation packages [4]. 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. For constrained systems, BLieDF2nd is combined with the index-3 formulation of the equations of motion [4]. We prove convergence with order $p = k$ in all solution components for BLieDF2nd with $2 \leq k \leq 4$ and illustrate the theoretical investigations by numerical tests for unconstrained and constrained versions of the heavy top benchmark.

BDF and the update of solution increments BDF are k-step methods that are zero-stable for $k \leq 6$ and achieve global order of accuracy $p = k$. For ODEs $\dot{\mathbf{x}} = \mathbf{f}(t,\mathbf{x})$, the numerical solution $\mathbf{x}_{n+1}$ at $t = t_{n+1} = t_n + h$ is defined implicitly by the corrector equations

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

with h denoting the (fixed) time step size and algorithmic parameters $\alpha_0, \alpha_1, \ldots, \alpha_k$ satisfying $\sum_i \alpha_i = 0$. In this classical form (1), the multi-step method can not be applied to the Lie group setting since there are no linear combinations $\sum_i \alpha_i \mathbf{x}_{n+1-i}$ in a nonlinear configuration space. Therefore, we transform (1) to an equivalent formula in terms of solution increments resulting in the one-step update

$$\mathbf{x}_{n+1} = \mathbf{x}_n + h\,\Delta\mathbf{x}_n \tag{2a}$$

with a vector $\Delta\mathbf{x}_n$ that is defined implicitly by the new corrector equations

$$\sum_{i=1}^{k} \gamma_i \Delta\mathbf{x}_{n+1-i} = \mathbf{f}(t_{n+1}, \mathbf{x}_{n+1}) \text{ with } \gamma_1 := \alpha_0 \text{ and } \gamma_i := \sum_{j=0}^{i-1} \alpha_j\,,\ \Delta\mathbf{x}_{n+1-i} := \frac{\mathbf{x}_{n+2-i} - \mathbf{x}_{n+1-i}}{h}\,,\ (i = 2, \ldots, k)\,. \tag{2b}$$

BLieDF2nd We consider constrained systems being described by a 2nd order DAE on a Lie group G:

$$\dot{q} = DL_q(e) \cdot \widetilde{\mathbf{v}}\,, \tag{3a}$$

$$\mathbf{M}(q)\dot{\mathbf{v}} = -\mathbf{g}(q,\mathbf{v},t) - \mathbf{B}^{\top}(q)\boldsymbol{\lambda}\,, \tag{3b}$$

$$\Phi(q) = \mathbf{0} \tag{3c}$$

with configuration variables $q \in G$, velocity coordinate $\mathbf{v} \in \mathbb{R}^k$, Lagrange multipliers $\boldsymbol{\lambda}$, mass matrix $\mathbf{M}$, force vector $\mathbf{g}$, holonomic constraints (3c), constraint gradients $\mathbf{B}(q)$, the tilde operator $\widetilde{(\bullet)} : \mathbb{R}^k \to \mathfrak{g}$ with Lie algebra $\mathfrak{g}$ and directional derivative of the left translation $DL_q(e) : \mathfrak{g} \to T_qG, \widetilde{\mathbf{v}} \mapsto DL_q(e) \cdot \widetilde{\mathbf{v}}$ in e along $\widetilde{\mathbf{v}}$, see [1].

Following the Lie algebra approach [3], the kinematic equations (3a) are discretized by a (*nonlinear*) Lie group version of (2a) with solution increments $\Delta\mathbf{q}_n \in \mathfrak{g}$ in a *linear* space. Instead of time-consuming re-parametrizations of the configuration space, we just use exponential map $\exp : \mathfrak{g} \to G$ and Lie group operation $\circ : G \times G \to G$:

$$q_{n+1} = q_n \circ \exp(h\widetilde{\Delta\mathbf{q}}_n)\,, \tag{4a}$$

$$\sum_{i=1}^{k} \gamma_i \Delta\mathbf{q}_{n+1-i} = \mathbf{v}_{n+1} + h^2\mathbf{L}_k(\mathbf{v}_n, \mathbf{v}_{n-1}, \ldots, \mathbf{v}_{n-k}; h)\,, \tag{4b}$$

$$\frac{1}{h}\,\mathbf{M}(q_{n+1})\sum_{i=0}^{k} \alpha_i \mathbf{v}_{n+1-i} = -\mathbf{g}(t_{n+1}, q_{n+1}, \mathbf{v}_{n+1}) - \mathbf{B}^\top(q_{n+1})\boldsymbol{\lambda}_{n+1}\,, \tag{4c}$$

$$\Phi(q_{n+1}) = \mathbf{0} \tag{4d}$$

(details of initialization [4] are omitted because of space limitations). Note the correction term $h^2\mathbf{L}_k$ in the increment update (4b) that was introduced to avoid order reduction. Without this correction term, the order of convergence may drop to $p = \min\{k, 2\}$ as can be seen by the numerical test results in the upper left plot of Fig. 1 ("brute force approach"). Guided by the convergence analysis, we define

$$\mathbf{L}_2 \equiv \mathbf{0} \quad \text{and} \quad \mathbf{L}_3 = \mathbf{L}_3(\mathbf{v}_n, \mathbf{v}_{n-1}, \mathbf{v}_{n-2}; h) := \frac{1}{12}\hat{\mathbf{v}}_n\dot{\mathbf{v}}_n \quad \text{with} \quad \dot{\mathbf{v}}_n := \frac{3\mathbf{v}_n - 4\mathbf{v}_{n-1} + \mathbf{v}_{n-2}}{2h} \tag{5}$$

with the hat operator representing a matrix commutator in the sense of $\widetilde{\hat{\mathbf{v}}_n\dot{\mathbf{v}}_n} = [\widetilde{\mathbf{v}}_n, \widetilde{\dot{\mathbf{v}}}_n]$. The formal proof of global accuracy of order $p = k$ for BLieDF2nd with $k \leq 3$ is nicely illustrated by the numerical test results for unconstrained and constrained versions of the heavy top benchmark [1], see Fig. 1.

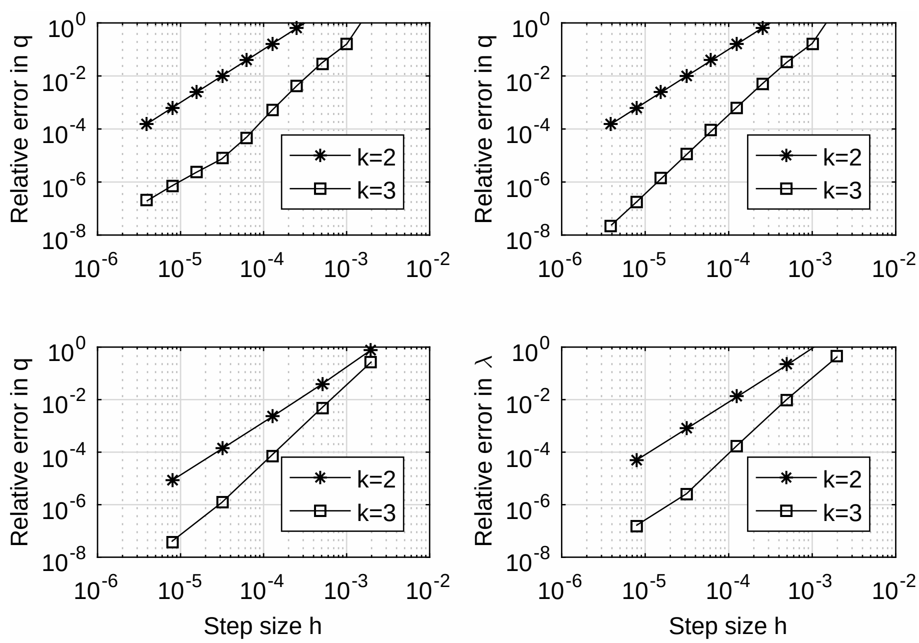

Fig. 1: BLieDF2nd for the heavy top benchmark [1]. Upper plots: unconstrained formulation with $\mathbf{L}_k \equiv \mathbf{0}$ (left plot, "brute force approach") and with $\mathbf{L}_k$ according to (5) (right plot). Lower plots: constrained formulation (left plot: error in q, right plot: error in $\boldsymbol{\lambda}$).

References

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