Half-explicit Runge-Kutta methods for constrained systems on Lie groups

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EXTENDED ABSTRACT

1 Introduction

Multibody systems with small deviations from a nominal state may be described conveniently in linear spaces parametrizing rotations, e.g., by Euler angles. On the other hand, nonlinear configuration spaces are the more natural choice for systems with large rotations since they allow a parametrization of rotations without singularities.

Typical examples are the group $\mathrm{SO}(3) \subset \mathbb{R}^{3\times 3}$ of rotation matrices, its direct or semi-direct products with $\mathbb{R}^3$ and Cartesian products $\big(\mathrm{SO}(3)\times\mathbb{R}^3\big)^k$ and $\big(\mathrm{SE}(3)\big)^k$ with the special Euclidean group $\mathrm{SE}(3) := \mathrm{SO}(3) \ltimes \mathbb{R}^3$. Isomorphic representations in terms of (unit) quaternions may improve the computational efficiency. All these nonlinear configuration spaces are equipped with a group operation "$\circ$" that combines basically the sum of position vectors with the matrix multiplication in $\mathrm{SO}(3)$. With this group operation, the nonlinear configuration space is not just a (differentiable) manifold but a Lie group, denoted by G.

Joints restrict the relative motion of bodies. If they are modelled by (holonomic) constraints then possible configurations are limited to a submanifold of G. Mathematically, constraint equations and the Lie group structure of G result both in a (sub-)manifold setting for the configuration space but they represent two completely different modelling aspects. Lie group DAE methods like the generalized-α Lie group method [2] consider these different aspects combining Lie group time integration [4] with solution techniques for constrained mechanical systems from the field of differential-algebraic equations (DAEs) in linear spaces [3].

The brute force approach to numerical methods on manifolds relies on local parametrizations. Munthe-Kaas proposed to update these local parametrizations in each time step and to solve (an approximation of) the corresponding ordinary differential equation (ODE) in terms of the local coordinates by one time step of a classical ODE method [4]. For typical configuration spaces in multibody system dynamics, the local parametrizations and the ODEs for local coordinates may be evaluated in closed form by Rodrigues like formulae for the exponential map exp, its (left) trivialized tangent $\mathrm{dexp}_{-\tilde{\mathbf{w}}}$ and the inverse $\mathrm{dexp}^{-1}_{-\tilde{\mathbf{w}}}$, see [6].

2 Half-explicit Runge-Kutta methods in the local coordinates approach

Recently, there has been new interest in the local coordinates approach to Lie group time integration [5, 7]. The present paper contributes a novel half-explicit Lie group integrator to this field of research. We consider equations of motion [2]

$$\dot{q} = DL_q(e)\cdot\tilde{\mathbf{v}}\,, \qquad \mathbf{M}(q)\dot{\mathbf{v}} + \mathbf{g}(q,\mathbf{v},t) + \mathbf{B}^\top(q)\,\boldsymbol{\lambda} = \mathbf{0}\,, \qquad \boldsymbol{\Phi}(q) = \mathbf{0} \tag{1}$$

with $q \in G$ representing the configuration of the system and $\mathbf{v} \in \mathbb{R}^n$ denoting the velocity vector. The most simple nontrivial example of this Lie group setting is given by $G = \mathrm{SO}(3)$ with 3×3 rotation matrices $q(t) = \mathbf{R}(t) \in G$, kinematic equations $\dot{\mathbf{R}} = \mathbf{R}\tilde{\boldsymbol{\omega}}$, angular velocity $\boldsymbol{\omega} = \mathbf{v} \in \mathbb{R}^3$ and $\tilde{\boldsymbol{\omega}} \in \mathfrak{so}(3)$ being defined by $\tilde{\boldsymbol{\omega}}\mathbf{w} = \boldsymbol{\omega}\times\mathbf{w}$, ($\mathbf{w} \in \mathbb{R}^3$).

Equations of motion (1) with a symmetric, positive definite mass matrix $\mathbf{M}(q)$ form a Lie group DAE of index 3. The r holonomic constraints $\boldsymbol{\Phi}(q) = \mathbf{0}$ are coupled to the dynamical equations by constraint forces $-\mathbf{B}^\top(q)\,\boldsymbol{\lambda}$ with Lagrange multipliers $\boldsymbol{\lambda} \in \mathbb{R}^r$ and a full-rank matrix $\mathbf{B}(q) \in \mathbb{R}^{r\times n}$ that represents the constraint gradients in the sense of $D\boldsymbol{\Phi}(q)\cdot\big(DL_q(e)\cdot\tilde{\mathbf{w}}\big) = \mathbf{B}(q)\mathbf{w}$ for all $\mathbf{w} \in \mathbb{R}^n$. For time integration, we substitute in (1) the constraints $\boldsymbol{\Phi}(q) = \mathbf{0}$ by their time derivative and get the analytically equivalent index-2 formulation of the equations of motion with constraints at the level of velocity coordinates

$$\mathbf{0} = \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Phi}\big(q(t)\big) = D\boldsymbol{\Phi}\big(q(t)\big)\cdot\dot{q}(t) = D\boldsymbol{\Phi}\big(q(t)\big)\cdot\big(DL_{q(t)}(e)\cdot\tilde{\mathbf{v}}(t)\big) = \mathbf{B}\big(q(t)\big)\mathbf{v}(t)\,. \tag{2}$$

In a neighbourhood of $t = t_m$, Lie group G is parametrized by elements $\tilde{\boldsymbol{\theta}}_m$ of the corresponding Lie algebra with local coordinates $\boldsymbol{\theta}_m \in \mathbb{R}^n$ that are known as incremental rotation vector in the case of $G = \mathrm{SO}(3)$. We get $q(t) = q(t_m)\circ\exp\big(\tilde{\boldsymbol{\theta}}_m(t)\big)$ with $\boldsymbol{\theta}_m(t)$ solving the locally defined initial value problem

$$\dot{\boldsymbol{\theta}}_m(t) = \mathbf{T}^{-1}\big(\boldsymbol{\theta}_m(t)\big)\,\mathbf{v}(t)\,,\ (\,t \geq t_m\,)\,,\ \ \boldsymbol{\theta}_m(t_m) = \mathbf{0} \tag{3}$$

that is written in matrix-vector form using the tangent operator $\mathbf{T}(\mathbf{w}) \in \mathbb{R}^{n\times n}$ for representing the left trivialized tangent $\mathrm{dexp}_{-\tilde{\mathbf{w}}}$ of the exponential map [4]. The time step $t_m \to t_{m+1} = t_m + h$ starts with numerical solutions $q_m \approx q(t_m)$, $\mathbf{v}_m \approx \mathbf{v}(t_m)$, $\boldsymbol{\lambda}_m \approx \boldsymbol{\lambda}(t_m)$ that define stage values $Q_{m1} = q_m\circ\exp(\tilde{\boldsymbol{\Theta}}_{m1})$ with $\boldsymbol{\Theta}_{m1} := \boldsymbol{\theta}_m(t_m) = \mathbf{0}$ and $\mathbf{V}_{m1} = \mathbf{v}_m$. The other stage values are given by

$$Q_{mi} = q_m\circ\exp(\tilde{\boldsymbol{\Theta}}_{mi})\,, \quad \boldsymbol{\Theta}_{mi} = h\sum_{j=1}^{i-1} a_{ij}\,\dot{\boldsymbol{\Theta}}_{mj}\,, \quad \mathbf{V}_{mi} = \mathbf{v}_m + h\sum_{j=1}^{i-1} a_{ij}\,\dot{\mathbf{V}}_{mj}\,,\ \ (\,i = 2,\ldots,\bar{s}+1\,)\,, \tag{4a}$$

with

$$\dot{\boldsymbol{\Theta}}_{mi} = \mathbf{T}^{-1}(\boldsymbol{\Theta}_{mi})\,\mathbf{V}_{mi}\,, \quad \mathbf{M}(Q_{mi})\dot{\mathbf{V}}_{mi} + \mathbf{g}(Q_{mi},\mathbf{V}_{mi},t_m+c_ih) + \mathbf{B}^{\top}(Q_{mi})\,\boldsymbol{\Lambda}_{mi} = \mathbf{0}\,, \;\; (i=1,\ldots,\bar{s})\,, \tag{4b}$$

suitable Runge-Kutta parameters a_{ij} and nodes $c_i := \sum_j a_{ij}$. The first Runge-Kutta stage has to be explicit in terms of $\boldsymbol{\Lambda}_{m1} := \boldsymbol{\lambda}_m$ to avoid order reduction and large local error terms [1]. In all other stages, we follow the approach of Brasey and Hairer [3] and enforce the hidden constraints (2) for the stage values $Q_{m,i+1}, \mathbf{V}_{m,i+1}$ such that each pair of stage vectors $(\dot{\mathbf{V}}_{mi}, \boldsymbol{\Lambda}_{mi})$, $(i=2,\ldots,\bar{s})$, is defined by a system of $n+r$ linear equations being composed of n dynamical equations in (4b) and r constraint equations:

$$\mathbf{0} = \mathbf{B}(Q_{m,i+1})\mathbf{V}_{m,i+1} = \mathbf{B}(Q_{m,i+1})\big(\mathbf{v}_m + h\sum_{j=1}^{i-1} a_{i+1,j}\,\dot{\mathbf{V}}_{mj} + h\,a_{i+1,i}\,\dot{\mathbf{V}}_{mi}\big)\,,\; (i=2,\ldots,\bar{s})\,. \tag{4c}$$

Finally, the numerical solution at $t=t_{m+1}$ is defined by $q_{m+1} = Q_{m,s+1}$, $\mathbf{v}_{m+1} = \mathbf{V}_{m,s+1}$ for a suitable $s \le \bar{s}$, i.e., by the explicit update (4a) with $i=s+1$ and parameters $a_{s+1,j}$ as Runge-Kutta weights that are often denoted by b_j, $(j=1,\ldots,s)$. For the Lagrange multipliers, the numerical solution is set to $\boldsymbol{\lambda}_{m+1} := \boldsymbol{\Lambda}_{m\bar{s}}$ or, more general, to $\boldsymbol{\lambda}_{m+1} := \sum_j d_j \boldsymbol{\Lambda}_{mj}$ with scalar parameters d_j, $(j=1,\ldots,\bar{s})$, that have to satisfy a contractivity condition to guarantee zero-stability of the half-explicit method [1, 3].

3 Numerical test results

The local coordinates approach results in Lie group methods that achieve their classical order known from ODE/DAE theory [4]. There are half-explicit Runge-Kutta Lie group methods of order $p=s$ for all $p \le 4$. Most attractive might be the half-explicit HEDOP5 integrator that is based on the explicit Runge-Kutta method of Dormand and Prince (known, e.g., as Matlab's default integrator `ode45`). HEDOP5 has $s=6$, $\bar{s}=8$ stages and converges with order $p=5$ in all solution components [1, 3].

Fig. 1 shows numerical test results for three half-explicit Runge-Kutta Lie group methods being applied with fixed time step sizes to the heavy top benchmark [2] that is formulated as a constrained system in SE(3). All three methods achieve the theoretically predicted order of convergence with the 5th order method HEDOP5 being clearly superior to the two lower order methods.

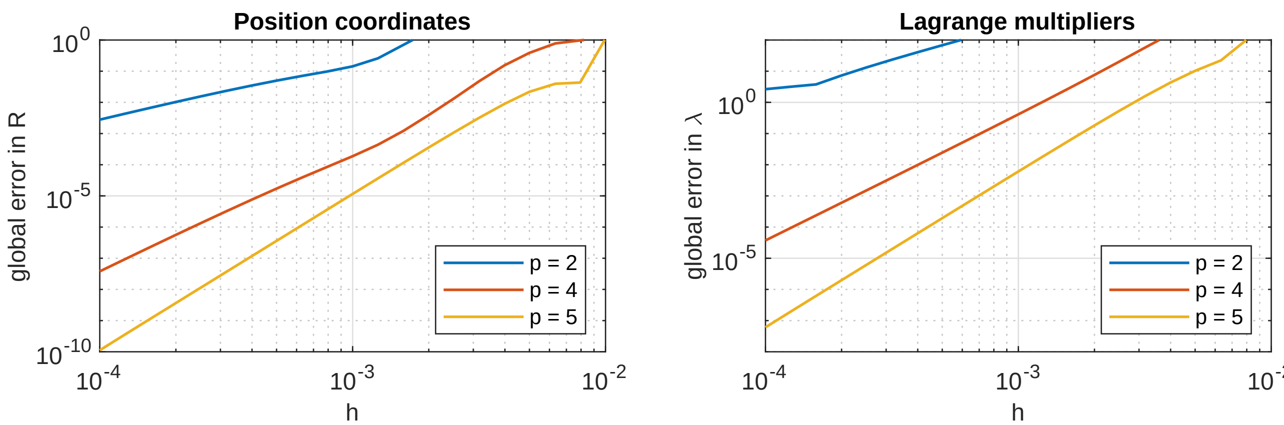

Figure 1: Global error of half-explicit Runge-Kutta Lie group methods for heavy top benchmark in SE(3).

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