EasyChair Preprint

№ XXX

Stability analysis of Lie group integrators in terms of test equations

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May 22, 2024

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1 Introduction

Multibody systems with large rotations may be described conveniently and free of singularities in non-linear configuration spaces with Lie group structure. Lie group integrators preserve this structure in the sense that the numerical solution will remain (by construction) in the Lie group. The methods go back to the work of Crouch and Grossman (1993) and Munthe-Kaas (1998), see [5], and have become one of the standard approaches in flexible multibody dynamics with the seminal paper of Brüls and Cardona (2010) on Lie group time integration for constrained systems [2].

Today, virtually any classical time integration method from system dynamics has its Lie group counterpart including implicit and (half-)explicit methods, methods for constrained and for unconstrained systems, variational integrators, one-step and multistep methods, Newmark type methods etc. There is not much known about the numerical stability of these methods in the application to stiff systems.

More precisely, one would be interested in criteria and step size bounds that guarantee that the distance between two numerical solutions for different initial values remains bounded on infinite time intervals. In linear spaces, such error bounds are known, e.g., from the theory of B-stability for systems that satisfy a one-sided Lipschitz condition [4].

For differential equations on Riemannian manifolds, a first stability result of that type was presented by Owren at the FoCM 2023 conference in Paris. He proves B-stability of the geodesic implicit Euler method on Riemannian manifolds with non-positive sectional curvature [1, Theorem 3.1]. In the present paper, we follow a different path and focus on the application of Lie group integrators to test problems from rigid body dynamics.

2 Test equations in linear spaces

This work was inspired by the classical Dahlquist equation $\dot{y} = \lambda y$ with a parameter $\lambda \in \mathbb{C}^-$. The Dahlquist equation results, e.g., from the equation

$$m\ddot{\xi} + d\dot{\xi} + k\xi = 0 \tag{$*$}$$

of an oscillating point mass m with stiffness and damping parameters $k > 0$, $d \geq 0$ if the equivalent first order system in terms of $(\xi, \dot{\xi})$ is transformed to two decoupled equations $\dot{y}_i = \lambda_i y_i$, $(i = 1, 2)$, with $\lambda_{1,2} = (-d \pm \sqrt{d^2 - 4km})/2m$ and $y_1 := \lambda_2 \xi - \dot{\xi}$, $y_2 := \dot{\xi} - \lambda_1 \xi$.

The scalar test equation $(*)$ represents all linear time-invariant systems $\mathbf{M}\ddot{\mathbf{x}} + \mathbf{D}\dot{\mathbf{x}} + \mathbf{K}\mathbf{x} = \mathbf{0}$ with symmetric positive definite mass and stiffness matrices $\mathbf{M}, \mathbf{K} \in \mathbb{R}^{n \times n}$ and Rayleigh damping in terms of $\mathbf{D} = c_{\mathbf{M}}\mathbf{M} + c_{\mathbf{K}}\mathbf{K}$ with constants $c_{\mathbf{M}}, c_{\mathbf{K}} \geq 0$: In a first step, the mass matrix $\mathbf{M}$ is diagonalized by orthogonal transformations resulting in $\mathbf{M} = \mathbf{U_M}\,\mathbf{\Lambda_M}\,\mathbf{U_M}^\top$ with $\mathbf{\Lambda_M} = \mathrm{diag}_i\, m_i$. Then, a second orthogonal transformation $\mathbf{\Lambda_M}^{-1/2}\,\mathbf{U_M}^\top \mathbf{K}\,\mathbf{U_M}\,\mathbf{\Lambda_M}^{-1/2} = \mathbf{U_\Omega}\big(\mathbf{\Lambda_M}^{-1/2}\,\mathbf{\Lambda_K}\,\mathbf{\Lambda_M}^{-1/2}\big)\mathbf{U_\Omega}^\top$ with $\mathbf{\Lambda_K} = \mathrm{diag}_i\, k_i$ results in n scalar equations $m_i\ddot{\xi}_i + d_i\dot{\xi}_i + k_i\xi_i = 0$, $(i = 1, \ldots, n)$, in terms of $(\xi_1, \ldots, \xi_n)^\top = \mathbf{\Lambda_M}^{-1/2}\,\mathbf{U_\Omega}^\top\,\mathbf{\Lambda_M}^{1/2}\,\mathbf{U_M}^\top\,\mathbf{x}$ with $d_i = c_{\mathbf{M}} m_i + c_{\mathbf{K}} k_i$, see $(*)$. I.e., the A-stability analysis for the scalar Dahlquist test equation and the equation $(*)$ for the oscillating point mass with a damped linear spring give insight for a rather large class of (linear) problems.

3 Test problem: Rotating ball with (damped) torsional spring

In a Lie group setting, the natural counterpart to the scalar system $m\ddot{\xi} + d\dot{\xi} + k\xi = 0$ is a (damped) torsional spring being attached to a rigid ball with homogeneous mass distribution that has its centre in the origin and rotates around a fixed axis $\mathbf{n} \in \mathbb{R}^3$, $\|\mathbf{n}\|_2 = 1$. In SO(3), the orientation of the body is given by $\mathbf{R} = \exp_{\mathrm{SO(3)}}(\alpha\,\tilde{\mathbf{n}})$ with $\alpha \in \mathbb{R}$ denoting the angle of rotation and the skew symmetric matrix $\tilde{\mathbf{n}} \in \mathbb{R}^{3\times 3}$ that represents the vector product in the sense of $\tilde{\mathbf{n}}\,\mathbf{w} = \mathbf{n} \times \mathbf{w}$, $(\mathbf{w} \in \mathbb{R}^3)$. The exponential map

is invertible in a neighbourhood of the origin and defines an inverse map $\widetilde{\log}_{\mathrm{SO}(3)} : \mathrm{SO}(3) \to \mathbb{R}^3$ with $\widetilde{\log}_{\mathrm{SO}(3)}\big(\exp_{\mathrm{SO}(3)}(\tilde{\boldsymbol{\theta}})\big) = \boldsymbol{\theta}$.
The ball's inertia tensor $\mathbf{J} = m\mathbf{I}_3$ results in gyroscopic terms that vanish identically: $\boldsymbol{\omega} \times \mathbf{J}\boldsymbol{\omega} = m\,\boldsymbol{\omega} \times \boldsymbol{\omega} = \mathbf{0}$. Here, $\boldsymbol{\omega} \in \mathbb{R}^3$ denotes the angular velocity that is parallel to the axis of rotation: $\boldsymbol{\omega} = v\,\mathbf{n}$ with $v \in \mathbb{R}$. With these notations, the torsional spring is characterized by a torque vector $-\big(d\,\boldsymbol{\omega} + k\,\widetilde{\log}_{\mathrm{SO}(3)}(\mathbf{R})\big) = -(dv + k\alpha)\,\mathbf{n}$ with damping and stiffness parameters d, k and yields equations of motion [3, Section 2.1]

$$\dot{\mathbf{R}} = \mathbf{R}\,\tilde{\boldsymbol{\omega}}\,, \quad \mathbf{J}\dot{\boldsymbol{\omega}} + d\,\boldsymbol{\omega} + k\,\widetilde{\log}_{\mathrm{SO}(3)}(\mathbf{R}) = \mathbf{0} \tag{1}$$

in the tangent bundle $T\mathrm{SO}(3)$. For the local parametrization based approach of Munthe-Kaas [5, Section 3], we consider incremental rotation vectors $\boldsymbol{\theta}_r(t) \in \mathbb{R}^3$ that parametrize $\mathbf{R}(t) = \exp_{\mathrm{SO}(3)}\big(\tilde{\boldsymbol{\theta}}_r(t)\big)\,\mathbf{R}(t_r)$ and solve a locally defined initial value problem

$$\dot{\boldsymbol{\theta}}_r(t) = \big(T_{\mathrm{SO}(3)}(\boldsymbol{\theta}_r(t))\big)^{-1}\,\boldsymbol{\omega}(t)\,, \quad \boldsymbol{\theta}_r(t_r) = \mathbf{0} \tag{2}$$

with the tangent operator $T_{\mathrm{SO}(3)}$ of $\exp_{\mathrm{SO}(3)}$, see [2]. This operator represents the $\mathrm{dexp}_{\tilde{\boldsymbol{\theta}}_r}$ operator [5] in matrix form. Taking into account that $T_{\mathrm{SO}(3)}\big(s(t)\,\mathbf{n}\big)\,\big(\dot{s}(t)\,\mathbf{n}\big) = \dot{s}(t)\,\mathbf{n}$ for any scalar function $s(t)$, the solution of (2) with $\boldsymbol{\omega}(t) = v(t)\,\mathbf{n}$ is given by $\boldsymbol{\theta}_r(t) = s_r(t)\,\mathbf{n}$ with $\dot{s}_r(t) = v(t)$ and $s_r(t_r) = 0$, i.e., $\mathbf{R}(t) = \exp_{\mathrm{SO}(3)}\big(\alpha(t)\,\tilde{\mathbf{n}}\big)$ with $\dot{\alpha}(t) = \dot{s}_r(t) = v(t)$, $\dot{\alpha}(t)\,\mathbf{n} = \boldsymbol{\omega}(t)$, $\ddot{\alpha}(t)\,\mathbf{n} = \dot{\boldsymbol{\omega}}(t)$ and $0 = m\ddot{\alpha} + dv + k\alpha = m\ddot{\alpha} + d\dot{\alpha} + k\alpha$, see (1).
Time step $t_r \to t_{r+1} = t_r + h$ of a Runge-Kutta Munthe-Kaas method [5] defines $\mathbf{R}_{r+1} = \exp_{\mathrm{SO}(3)}(\tilde{\boldsymbol{\theta}}_r^+)\,\mathbf{R}_r$ with $\boldsymbol{\theta}_r^+ = h\sum_j b_j \dot{\boldsymbol{\theta}}_{rj}$ and $\boldsymbol{\omega}_{r+1} = \boldsymbol{\omega}_r^+ = \boldsymbol{\omega}_r + h\sum_j b_j \dot{\boldsymbol{\omega}}_{rj}$. The stage vectors are $\boldsymbol{\omega}_{ri} = \boldsymbol{\omega}_r + h\sum_j a_{ij}\dot{\boldsymbol{\omega}}_{rj}$, $\boldsymbol{\theta}_{ri} = h\sum_j a_{ij}\dot{\boldsymbol{\theta}}_{rj}$,

$$\dot{\boldsymbol{\omega}}_{ri} = -\mathbf{J}^{-1}\big(d\,\boldsymbol{\omega}_{ri} + k\,\widetilde{\log}_{\mathrm{SO}(3)}(\mathbf{R}_{ri})\big)\,, \quad \mathbf{R}_{ri} = \exp_{\mathrm{SO}(3)}(\tilde{\boldsymbol{\theta}}_{ri})\,\mathbf{R}_r\,, \quad \dot{\boldsymbol{\theta}}_{ri} = \big(T_{\mathrm{SO}(3)}(\boldsymbol{\theta}_{ri})\big)^{-1}\,\boldsymbol{\omega}_{ri}\,, \tag{3}$$

$(i = 1, \ldots, s)$. As for the analytical solution $\big(\boldsymbol{\theta}_r(t), \boldsymbol{\omega}(t)\big)$ and its time derivative, we see that all stage vectors $\boldsymbol{\theta}_{ri}, \dot{\boldsymbol{\theta}}_{ri}, \boldsymbol{\omega}_{ri}, \dot{\boldsymbol{\omega}}_{ri}$ are parallel to $\mathbf{n}$ resulting in numerical solutions $\mathbf{R}_{r+1} = \exp_{\mathrm{SO}(3)}\big(\alpha_{r+1}\,\tilde{\mathbf{n}}\big)$ and $\boldsymbol{\omega}_{r+1} = v_{r+1}\,\mathbf{n}$ with (α_{r+1}, v_{r+1}) being the result of a classical Runge-Kutta step for the first order system $\dot{\alpha} = v$, $m\dot{v} = -dv - k\alpha$ starting from (α_r, v_r). For this test problem, the Runge-Kutta Lie group integrator shares one-by-one the well known stability properties of its classical counterpart applied to the second order problem in linear spaces.
Initial values $\boldsymbol{\omega}(t_0)$ being *not* parallel to vector $\mathbf{n}$ may cause a more complex behaviour of Lie group integrators that will be illustrated by a series of numerical test results.

Acknowledgments The author acknowledges gratefully fruitful discussions with Elena Celledoni, Ergys Çokaj, Brynjulf Owren (Trondheim) and Denise Tumiotto (Halle) on contractivity of Lie group time integration methods.

That research has been part of the THREAD project, see `https://thread-etn.eu/`, that has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 860124.

The present paper reflects only the authors' view and the European Commission's Research Executive Agency is not responsible for any use that may be made of the information it contains.

References

[1] M. Arnold, E. Celledoni, E. Çokaj, B. Owren, and D. Tumiotto. B-stability of numerical integrators on Riemannian manifolds. arXiv:2308.08261 [math.NA], August 2023.

[2] O. Brüls and A. Cardona. On the use of Lie group time integrators in multibody dynamics. *ASME J. Comput. Nonlinear Dynam.*, 5:031002 (13 pages), 2010.

[3] O. Brüls, A. Cardona, and M. Arnold. Lie group generalized-α time integration of constrained flexible multibody systems. *Mechanism and Machine Theory*, 48:121–137, 2012.

[4] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations. II. Stiff and Differential-Algebraic Problems*. Springer–Verlag, Berlin Heidelberg New York, 2nd edition, 1996.

[5] A. Iserles, H.Z. Munthe-Kaas, S. Nørsett, and A. Zanna. Lie-group methods. *Acta Numerica*, 9:215–365, 2000.