DETC2013-12308

DRAFT: STÖRMER–VERLET INTEGRATION SCHEME FOR MULTIBODY SYSTEM DYNAMICS IN LIE-GROUP SETTING

Zdravko Terze
Department of Aeronautical Engineering
Faculty of Mechanical Engineering and Naval Architecture
University of Zagreb
10002 Zagreb, Croatia
Email: zdravko.terze@fsb.hr

Andreas Mueller
Institute of Mechatronics
09126 Chemnitz, Germany
Email: andreas.mueller@ifm-chemnitz.de

Dario Zlatar
Department of Aeronautical Engineering
Faculty of Mechanical Engineering and Naval Architecture
University of Zagreb
10002 Zagreb, Croatia
Email: dario.zlatar@fsb.hr

ABSTRACT

Störmer-Verlet integration scheme has many attractive properties when dealing with ODE systems in linear spaces: it is explicit, 2nd order, linear/angular momentum preserving and it is symplectic for Hamiltonian systems. In this paper we investigate its application for numerical simulation of the multibody system dynamics (MBS) by formulating Störmer-Verlet algorithm for the constrained mechanical systems with the direct rotation group $SO(3)$ upgrade in Lie-group setting. Starting from the investigations on the single rigid body rotational dynamics, the paper introduces modified RATTLE integration scheme with the $SO(3)$ rotational upgrade that is designed via exponential map and utilization of the rotation group Lie-algebra $so(3)$, which is determined from the canonical coordinate of Hamiltonian system during integration of the system dynamics.

CONFIGURATION SPACE AND BASIC FORMULATION

In the adopted approach, the configuration space of MBS comprising k bodies is modeled as a Lie-group $G = \mathcal{R}^3 \times ... \times \mathcal{R}^3 \times SO(3) \times ... \times SO(3)$ (k copies of $\mathcal{R}^3 \times SO(3)$) with the elements of the form $p = (\mathbf{x}_1,...,\mathbf{x}_k, \mathbf{R}_1,...,\mathbf{R}_k)$. Each factor $\mathcal{R}^3 \times SO(3)$ represents a configuration of the one single rigid body represented by $(\mathbf{x}_i, \mathbf{R}_i)$ - its position vector and the rotation matrix w.r.t. a global frame (for rigid body i). G is a Lie-group of the dimension $n = 6k$ where k is the number of the rigid bodies.

The angular velocity of a rigid body is given by the left-invariant vector field $\widetilde{\omega}_i \in so(3)$ defined as $\dot{\mathbf{R}}_i(t) = \mathbf{R}_i(t)\widetilde{\omega}_i$ with $so(3)$ being the Lie algebra of $SO(3)$. A velocity of the one body (rigid body i) can thus be represented by the couple $(\mathbf{v}_i, \omega_i) \in \mathcal{R}^3 \times so(3)$.

Aiming on the application of the Lie-group integration scheme, also the MBS state space must be expressed as a Lie-group. Therefore, the MBS state space $S = \mathcal{R}^3 \times ... \times \mathcal{R}^3 \times SO(3) \times ... \times SO(3) \times \mathcal{R}^3 \times ... \times \mathcal{R}^3 \times so(3) \times ... ... \times so(3) \cong TG$ is introduced, with the elements $q = (\mathbf{x}_1,...,\mathbf{x}_k, \mathbf{R}_1,...,\mathbf{R}_k, \mathbf{v}_1,...,\mathbf{v}_k, \omega_1,...,\omega_k)$. This is a Lie-group itself and possess the Lie-algebra $\mathbf{s} = \mathcal{R}^3 \times ... \times \mathcal{R}^3 \times so(3) \times ... \times so(3) \times \mathcal{R}^3 \times ... \times \mathcal{R}^3 \times \mathcal{R}^3 \times ... \times \mathcal{R}^3$ with the element $z = (\mathbf{v}_1,...,\mathbf{v}_k, \widetilde{\omega}_1,...,\widetilde{\omega}_k, \dot{\mathbf{v}}_1,...,\dot{\mathbf{v}}_k, \dot{\omega}_1,...,\dot{\omega}_k)$. To formulate dynamical model of the constrained MBS in the introduced state space, the constrained Boltzmann-Hamel equations are used [1]

$$\mathbf{M}(p)\dot{\mathbf{v}} + \mathbf{C}^T(p)\lambda = \mathbf{Q}(p, \mathbf{v}, t)$$
$$\dot{p} = p \cdot \mathbf{v} \qquad (1)$$
$$\mathbf{\Phi}(p) = 0 \,,$$

where $\mathbf{M}$ is $n \times n$ dimensional generalized inertia matrix, $\mathbf{v} \in \mathcal{R}^n$, $\mathbf{v} = [\mathbf{v}_1,...,\mathbf{v}_k, \omega_1,...,\omega_k]^T$ are the system velocities (k bodies are assumed), $\mathbf{Q}$ represents the external and all other

forces, $\lambda \in \mathcal{R}^m$ is the vector of Lagrange multipliers and $\mathbf{C}$ is $m \times n$ dimensional constraint Jacobian, such that $\mathbf{\Phi}'(p) \cdot \tilde{\mathbf{v}} = \mathbf{C}(p)\mathbf{v}$, where $\mathbf{\Phi}'$ is the differential mapping of the constraint mapping $\mathbf{\Phi}: G \to \mathcal{R}^m$. Consequently, a MBS is constrained to evolve on the n-m dimensional sub-manifold $S = \{p \in G : \mathbf{\Phi}(p) = 0\}$. The equation $\dot{p} = p \cdot \tilde{\mathbf{v}}$ in (1) achieves the reconstruction of the motion from the velocities $\mathbf{v}$.

RIGID BODY INTEGRATION SCHEME WITH THE ROTATIONAL GROUP SO(3) DIRECT UPGRADE

To illustrate application of the Störmer-Verlet integration scheme [2], for the integration of the system configured as (1), the rotational dynamics of a rigid body (an essential and the most involved step within the overall MBS rigid body integration procedure) is studied in the sequel. With this aim in view, we model rigid body rotational dynamics as Hamiltonian system constrained to the Lie-group $SO(3)$, and evolving on the cotangent bundle $T^* SO(3)$.

If we introduce diagonal matrix $\mathbf{D} = \text{diag}(d_1, d_2, d_3)$ with the coefficients defined in (2), where the eigenvalues I_1, I_2, I_3 of the rigid body inertia tensor are given as

$$I_1 = d_2 + d_3,\ I_2 = d_3 + d_1,\ I_3 = d_1 + d_2,\ d_k = \int_{\mathcal{B}} x_k^2 dm(x), \quad (2)$$

the kinetic energy E_k of the system can be written as [8]

$$E_k = \frac{1}{2}\text{trace}(\tilde{\boldsymbol{\omega}}\mathbf{D}\tilde{\boldsymbol{\omega}}^T) = \text{trace}(\dot{\mathbf{R}}\mathbf{D}\dot{\mathbf{R}}^T), \quad (3)$$

where we use left trivialization equation $\dot{\mathbf{R}} = \mathbf{R}\tilde{\boldsymbol{\omega}}$ [3]. Introducing the conjugate momenta

$$\mathbf{P} = \frac{\partial E_k}{\partial \dot{\mathbf{R}}} = \dot{\mathbf{R}}\mathbf{D}, \quad (4)$$

we obtain the following system Hamiltonian where both $\mathbf{P}$ and $\mathbf{R}$ are 3×3 matrices

$$H(\mathbf{P}, \mathbf{R}) = \frac{1}{2}\text{trace}(\mathbf{P}\mathbf{D}^{-1}\mathbf{P}^T) + U(\mathbf{R}), \quad (5)$$

and where we suppose to have, in addition to E_k, an external potential $U(\mathbf{R})$. Then, the equation of motion for a rigid body, modeled as a constrained Hamiltonian system [5, 7], can be written as

$$\dot{\mathbf{R}} = \nabla_{\mathbf{P}}H(\mathbf{P}, \mathbf{R}) = \mathbf{P}\mathbf{D}^{-1}$$
$$\dot{\mathbf{P}} = -\nabla_{\mathbf{R}}H(\mathbf{P}, \mathbf{R}) - \mathbf{R}\boldsymbol{\Lambda} = -\nabla U(\mathbf{R}) - \mathbf{R}\boldsymbol{\Lambda} \quad (6)$$
$$0 = \mathbf{R}^T\mathbf{R} - \mathbf{I}$$

where we use the notations $\nabla U = (\partial U / \partial \mathbf{R}_{ij})$, $\nabla_{\mathbf{R}}H = (\partial H / \partial \mathbf{R}_{ij})$, and similarly for $\nabla_{\mathbf{P}}H$.

Here, the coefficients of the symmetric matrix $\boldsymbol{\Lambda}$ correspond to the six Lagrange multipliers associated to the constraint equation

$$\mathbf{R}^T\mathbf{R} - \mathbf{I} = 0, \quad (7)$$

that is due to the redundant formulation of the rigid body 3 DOF rotational kinematics. After differentiation of this constraint at the 'generalized position' level, we obtain 'velocity' constraint equation $\mathbf{R}^T\dot{\mathbf{R}} + \dot{\mathbf{R}}^T\mathbf{R} = 0$, which yields

$$\mathbf{R}^T\mathbf{P}\mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{P}^T\mathbf{R} = 0. \quad (8)$$

These two constraints imply that the equations (6) constitute a Hamiltonian system constrained on the manifold

$$\mathcal{K} = \left\{(\mathbf{P}, \mathbf{R}) \in \mathcal{R}^{3\times3} \times \mathcal{R}^{3\times3};\ \mathbf{R}^T\mathbf{R} = \mathbf{I},\ \mathbf{R}^T\mathbf{P}\mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{P}^T\mathbf{R} = 0\right\}.$$

Here, it should be emphasized that $\mathcal{K}$ is not cotangent bundle $T^* SO(3)$ associated to the manifold $SO(3)$.

By following [6, 9], we introduce Störmer-Verlet integration scheme for the constrained mechanical systems in the RATTLE form. In the contrast to the 'standard' RATTLE scheme [5, 6], we introduce the rotational upgrade on $SO(3)$ via Lie-group integration step, as indicated in the second equation of (9). With this operation in place, the RATTLE integrator for the rigid body rotational dynamics can be written in the form

$$\mathbf{P}_{1/2} = \mathbf{P}_0 - \frac{h}{2}\nabla U(\mathbf{R}_0) - \frac{h}{2}\mathbf{R}_0\boldsymbol{\Lambda}_0(\mathbf{P}, \mathbf{Q})$$
$$\mathbf{R}_1 = \mathbf{R}_0 \exp(h\mathbf{R}_0^T\mathbf{P}_{1/2}\mathbf{D}^{-1}) \quad (9)$$
$$\mathbf{P}_1 = \mathbf{P}_{1/2} - \frac{h}{2}\nabla U(\mathbf{R}_1) - \frac{h}{2}\mathbf{R}_1\boldsymbol{\Lambda}_1,\quad \mathbf{R}_1^T\mathbf{P}_1\mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{P}_1^T\mathbf{R}_1 = 0$$

where $\boldsymbol{\Lambda}_0$ and $\boldsymbol{\Lambda}_1$ are symmetric matrices. Unlike $\boldsymbol{\Lambda}_0$ (that, in this formulation, will be substituted by the expression $\boldsymbol{\Lambda}_0(\mathbf{P}, \mathbf{Q})$, derived via differentiation of (8) and explicit elimination of $\boldsymbol{\Lambda}_0$ in the first equation of (9)), $\boldsymbol{\Lambda}_1$ is the velocity constraint Lagrange multiplier that 'forces' solution of $\mathbf{P}_1$ to stay on the constraint manifold given by (8) - on technical terms, the calculation of the last two equations of (9) requires solving of linear algebraic systems for $\mathbf{P}_1$ and $\boldsymbol{\Lambda}_1$.

On the contrary to angular velocities, the satisfaction of the 'generalized position' constraint (7) within the algorithm is automatically assured by the exponential mapping operation incorporated into the second equation of (9).

As a numerical illustration of the algorithm, we consider the motion of freely spinning body [4]. The initial condition is body

angular velocity $\boldsymbol{\omega}_0 = \begin{bmatrix} 0.45549 & 0.82623 & 0.03476 \end{bmatrix}^T$ and inertia tensor with the diagonal elements $\mathbf{J} = \mathrm{diag}(0.9144, \; 1.098, \; 1.66)$.

A body angular velocity (expressed in the body coordinate system) and elements of the body rotation matrix $\mathbf{R} \in SO(3)$ are shown in Figure 1 and 2.
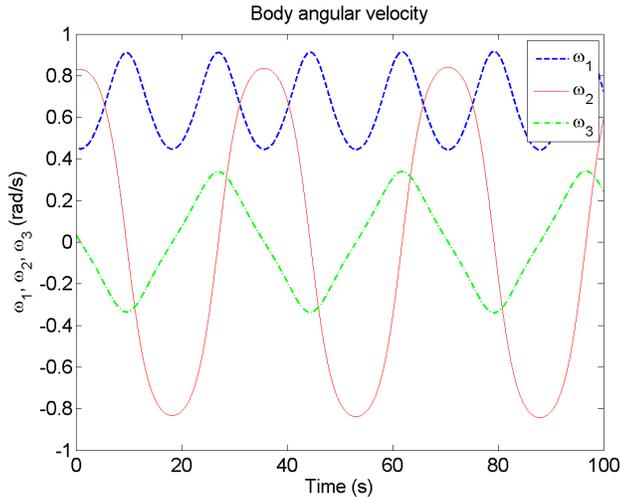
FIGURE 1. BODY ANGULAR VELOCITY.
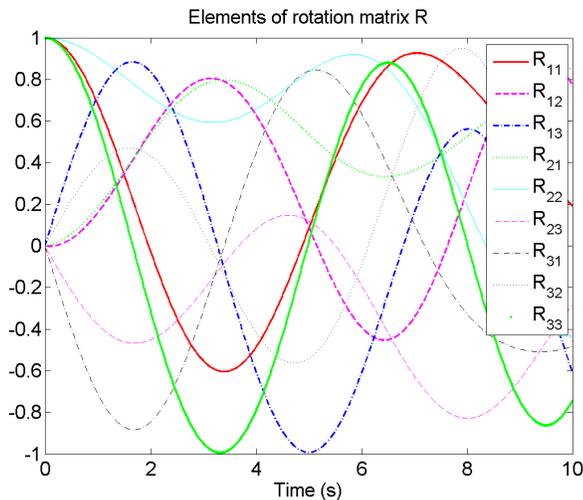
FIGURE 2. ELEMENTS OF ROTATION MATRIX $\mathbf{R}$.
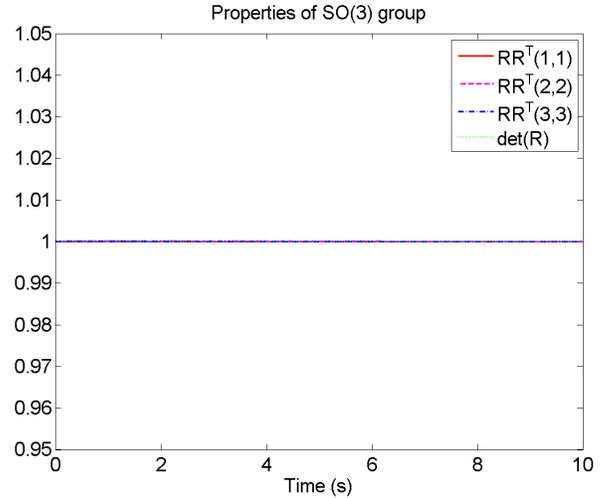
FIGURE 3. PROPERTIES OF ROTATION MATRIX $\mathbf{R} \in SO(3)$. DIAGONAL ELEMENTS OF PRODUCT $\mathbf{R}^T \mathbf{R} = \mathbf{I}$ AND DETERMINANT $\det \mathbf{R} = +1$.

The matrix entries along the main diagonal as well as the matrix determinant $(\mathbf{R}\mathbf{R}^T = \mathbf{I}, \det \mathbf{R} = +1)$ are presented in Figure 3.

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