Rigid body dynamics

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Rigid body dynamics

Synonyms

Euler's equations.

Short definition

Rigid body dynamics is the study of the motion in space of one or several bodies in which deformation is neglected.

Description

It was a surprising discovery of Euler (1758) that the motion of a rigid body $\mathcal{B}$ in $\mathbb{R}^3$ with an arbitrary shape and an arbitrary mass distribution is characterized by a differential equation involving only three constants, the moments of inertia, that we shall denote I_1, I_2, I_3– also called the Euler constants of the rigid body – and related to the principal axis of inertia of the body. Still, the description of the motion of a general non-symmetric rigid body is non trivial and possesses several geometric features. It arises in many fields such as solid mechanics or molecular dynamics. It is thus a target of choice for the design of efficient structure preserving numerical integrators. We refer to the monographs by Leimkuhler and Reich (2004, Chap. 8) and by Hairer et al (2006, Sect. VII.5) for a detailed survey of rigid body integrators in the context of geometric numerical integration (see also references therein) and to Marsden and Ratiu (1999) for a more abstract presentation of rigid body dynamics using the Lie-Poisson theory.

Equations of motion of a free rigid body

For the description of the rotation of a rigid body $\mathcal{B}$, we consider two frames: a fixed frame attached to the laboratory and a body frame attached to the rigid body itself and moving along time. We consider in Figure 1 the classical rigid body example of a hardbound book (see the body frame in the left picture). We represent the rotation axis in the body frame by a vector $\omega = (\omega_1, \omega_2, \omega_3)^T$ with components the speeds of rotation around each body axis. Its direction corresponds to the rotation axis and its length is the speed of rotation. The velocity of a point x in the body frame with respect to the origin of the body frame is given by the exterior product $v = \omega \times x$. Assume that the rigid body $\mathcal{B}$ has mass distribution dm. Then, the kinetic T energy is obtained by integrating over the body the energy of the mass point $dm(x)$,

$$T = \frac{1}{2} \int_{\mathcal{B}} \|\omega \times x\|^2 dm(x) = \frac{1}{2} \omega^T \Theta \omega,$$

where the symmetric matrix Θ, called the inertia tensor, is given by $\Theta_{ii} = \int_{\mathcal{B}} (x_j^2 + x_k^2) dm(x)$ and $\Theta_{ij} = -\int_{\mathcal{B}} x_i x_j dm(x)$ for all distinct indices i, j, k. The kinetic energy T is a quadratic form in ω, thus it can be reduced into a diagonal form in an orthonormal basis of the body. Precisely, if the body frame has its axes parallel to the eigenvectors of Θ – the principal axes of the rigid body, see the left picture of Figure 1 – then the kinetic energy takes the form

$$T = \frac{1}{2} \big(I_1 \omega_1^2 + I_2 \omega_2^2 + I_3 \omega_3^2 \big), \tag{1}$$

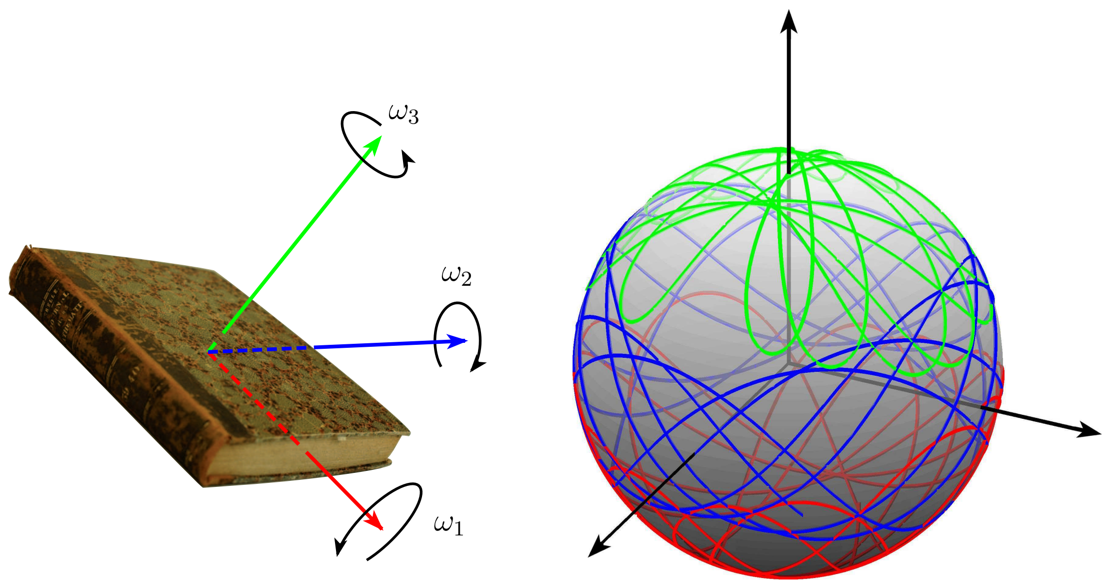

Fig. 1. Example of a a rigid body: the issue 39 of the Journal de Crelle where the article by Jacobi (1850) was published. Left picture: the rigid body and its three principal axis of inertia at the gravity center (coloured arrows). Right picture: free rigid body trajectories of the principal axis relative to the fixed frame (columns of Q with the corresponding colors). Computation with the preprocessed DMV algorithm of order 10 (see Alg. 4) with timestep $h = 0.01$, $0 \le t \le 40$, and initial condition $y(0) = (0, 0.6, -0.8)^T$, $Q(0) = I$. Moments of Inertia: $I_1 = 0.376, I_2 = 0.627, I_3 = 1.0$.

where the eigenvalues I_1, I_2, I_3 of the inertia tensor are called the moments of inertia of the rigid body. They are given by

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

Remark 1. Notice that for a rigid body that have interior points, we have $d_k > 0$ for all k. If one coefficient d_k is zero, then the body is flat, and if two coefficients d_k are zero, then the body is linear. For instance, the example in Fig.1 can be considered as a nearly flat body ($d_3 \ll d_1, d_2$).

Orientation matrix

The orientation at time t of a rigid body can be described by an orthogonal matrix $Q(t)$, which maps the coordinates $X \in \mathbb{R}^3$ of a vector in the body frame to the corresponding coordinates $x \in \mathbb{R}^3$ in the stationary frame via the relation $x = Q(t)X$. In particular, taking $X = e_k$, we obtain that the kth column of Q seen in the fixed frame corresponds to the unit vector e_k in the body frame, with velocity $\omega \times e_k$ in the body frame, and velocity $Q(\omega \times e_k)$ in the fixed frame. Equivalently, $\dot{Q}e_k = Q\widehat{\omega}e_k$ for all $k = 1, 2, 3$ and we deduce the equation for the orientation matrix $Q(t)$,

$$\dot{Q} = Q\widehat{\omega}. \tag{3}$$

Here, we shall use often the standard *hatmap* notation, satisfying $\widehat{\omega}x = \omega \times x$ (for all x), for the correspondence between skew-symmetric matrices and vectors in $\mathbb{R}^3$,

$$\widehat{\omega} = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}, \qquad \omega = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix}.$$

Since the matrix $Q^T\dot{Q} = \widehat{\omega}$ is skew-symmetric, we observe that the orthogonality $Q^TQ = I$ of the orientation matrix $Q(t)$ is conserved along time. As an illustration, we plot in right picture of Figure 1 the trajectories of the columns of Q, corresponding to orientation of the principal axis of the rigid body relative to fixed frame of the laboratory. It can be seen that even in the absence of an external potential, the solution for $Q(t)$ is non trivial (even though the solution $y(t)$ of the Euler equations alone is periodic).

Angular momentum

The angular momentum $y \in \mathbb{R}^3$ of the rigid body is obtained by integrating the quantity $x \times v$ over the body, $y = \int_{\mathcal{B}} x \times v \, dm(x)$, and using $v = x \times \omega$, a calculation yields the Poinsot relation $y = \Theta\omega$. Based on Newton's first law, it can be shown that in the absence of external forces the angular momentum is constant in the fixed body frame, i.e. the quantity $Q(t)y(t)$ is constant along time. Differentiating, we obtain $Q\dot{y} = -\dot{Q}y$, which yields $\dot{y} = -\omega \times y$. Considering the body frame with principal axis, the equations of motion of a rigid body in the absence of an external potential can now be written in terms of the angular momentum $y = (y_1, y_2, y_3)^T$, $y_j = I_j\omega_j$, as follows:

$$\frac{d}{dt}y = \widehat{y}\ J^{-1}y, \qquad \frac{d}{dt}Q = Q\ \widehat{J^{-1}y}, \tag{4}$$

where $J = \mathrm{diag}(I_1, I_2, I_3)$ is a diagonal matrix.

We notice that the flow of (4) has several first integrals. As mention earlier, Qy is conserved along time, and since Q is orthogonal, the Casimir

$$C(y) = \frac{1}{2}\Big(y_1^2 + y_2^2 + y_3^2\Big) \tag{5}$$

is also conserved. It also preserves the Hamiltonian energy

$$H(y) = \frac{1}{2}\Big(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\Big), \tag{6}$$

which is not surprising because the rigid body equations can be reformulated as a constrained Hamiltonian system as explained in the next section.

Remark 2. The left equation in (4) is called the Euler equations of the free rigid body. Notice that it can be written in the more abstract form of a Lie-Poisson system

$$\dot{y} = B(y)\nabla H(y)$$

where $H(y)$ is the Hamiltonian (6) and the skew-symmetric matrix $B(y) = \widehat{y}$ is the structure matrix of the Poisson system.[1] Notice that it cannot be cast as a canonical Hamiltonian system in $\mathbb{R}^3$ because $B(y)$ is not invertible.

Formulation as a constrained Hamiltonian system

The dynamics is determined by a Hamiltonian system constrained to the Lie group $SO(3)$, and evolving on the cotangent bundle $T^*SO(3)$. Consider the diagonal matrix $D = \mathrm{diag}(d_1, d_2, d_3)$ with coefficients defined in (2) which we assume to be nonzero for

[1] Indeed, the associated Lie-Poisson bracket is given by $\{F, G\}(y) = \nabla F(y)^T B(y)\nabla G(y)$ for two functions $F(y), G(y)$. It can be checked that it is anti-symmetric and it satisfies the Jacobi identity.

simplicity (see Remark 1). We observe that the kinetic energy T in (1) can be written as

$$T = \frac{1}{2}\,\mathrm{trace}(\widehat{w} D \widehat{w}^T) = \mathrm{trace}(\dot{Q} D \dot{Q}^T)$$

where we use (3) and $Q^T Q = I$. Introducing the conjugate momenta

$$P = \frac{\partial T}{\partial \dot{Q}} = \dot{Q} D,$$

we obtain the following Hamiltonian where both P and Q are 3×3 matrices

$$H(P, Q) = \frac{1}{2}\,\mathrm{trace}(P D^{-1} P^T) + U(Q)$$

and where we suppose to have, in addition to T, an external potential $U(Q)$. Then, the constrained Hamiltonian system for the motion of a rigid body writes

$$\begin{aligned}
\dot{Q} &= \nabla_P H(P, Q) = P D^{-1} \\
\dot{P} &= -\nabla_Q H(P, Q) - Q\Lambda = -\nabla U(Q) - Q\Lambda \quad (\Lambda \text{ symmetric}) \\
0 &= Q^T Q - I
\end{aligned} \tag{7}$$

where we use the notations $\nabla U = (\partial U / \partial Q_{ij})$, $\nabla_Q H = (\partial H / \partial Q_{ij})$, and similarly for $\nabla_P H$. Here, the coefficients of the symmetric matrix Λ correspond to the six Lagrange multipliers associated to the constraint $Q^T Q - I = 0$. Differentiating this constraint, we obtain $Q^T \dot{Q} + \dot{Q}^T Q = 0$, which yields $Q^T P D^{-1} + D^{-1} P^T Q = 0$. This implies that the equations (7) constitute a Hamiltonian system constraint on the manifold

$$\mathcal{P} = \{(P, Q) \in \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \;;\; Q^T Q = I, Q^T P D^{-1} + D^{-1} P^T Q = 0\}.$$

Notice that this is not the usual cotangent bundle associated to the manifold $SO(3)$, which can be written as

$$T^* SO(3) = \{(\overline{P}, Q) \in \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \;;\; Q^T Q = I, Q^T \overline{P} + \overline{P}^T Q = 0\},$$

but if we consider the symplectic change of variable $(P, Q) \mapsto (\overline{P}, Q)$ with $\overline{P} = P - Q\overline{\Lambda}$ and the symmetric matrix $\overline{\Lambda} = (Q^T P + P^T Q)/2$, then we obtain that the equations (7) define a Hamiltonian system on the cotangent bundle $T^*SO(3)$ in the variables $\overline{P}, Q$.

Lie-Poisson reduction

We observe from the identity

$$T = \frac{1}{2}\,\mathrm{trace}(PD^{-1}P^T) = \frac{1}{2}\,\mathrm{trace}(Q^T PD^{-1}(Q^T P)^T)$$

that the Hamiltonian T of the free rigid body depends on P, Q only via the quantity $Y = Q^T P$. We say that such Hamiltonian is left-invariant. It is a general result, see Marsden and Ratiu (1999) or Hairer et al (2006, Sect. VII.5.5), that such a left-invariant quadratic Hamiltonian on a Lie group can be reduced to a Lie-Poisson system (see Remark 2) in terms of $Y(t) = Q(t)^T P(t)$. Indeed, using the notation $\mathrm{skew}(A) = \frac{1}{2}(A - A^T)$, a calculation yields

$$\mathrm{skew}(\dot{Y}) = \mathrm{skew}(\dot{Q}^T P + Q^T \dot{P}) = \mathrm{skew}(D^{-1}Y^T Y) - \mathrm{skew}(Q^T \nabla U(Q))$$

Observing $2\,\mathrm{skew}(Y) = \hat{y}$, we deduce the reduced equations of motion of a rigid body in the presence of an external potential $U(Q)$,

$$\dot{y} = \widehat{y} J^{-1} y - \mathrm{rot}(Q^T \nabla U(Q)), \qquad \dot{Q} = Q\widehat{J^{-1}y}, \tag{8}$$

where for all square matrices M, we define $\widehat{\mathrm{rot}\, M} = M - M^T$. In the absence of an external potential ($U = 0$), notice that we recover the equations of motion of a free rigid body (4). We highlight that the reduced equations (8) are equivalent to (7) using the transformation $\hat{y} = Q^T P - P^T Q$. Written out explicitly, notice that the left part of (8) yields

$$\dot{y}_1 = \Big(\frac{1}{I_3} - \frac{1}{I_2}\Big) y_2 y_3 + \sum_{k=1}^{3} \Big(Q_{k2} \frac{\partial U(Q)}{\partial Q_{k3}} - Q_{k3} \frac{\partial U(Q)}{\partial Q_{k2}} \Big),$$
$$\dot{y}_2 = \Big(\frac{1}{I_1} - \frac{1}{I_3}\Big) y_3 y_1 + \sum_{k=1}^{3} \Big(Q_{k3} \frac{\partial U(Q)}{\partial Q_{k1}} - Q_{k1} \frac{\partial U(Q)}{\partial Q_{k3}} \Big),$$
$$\dot{y}_3 = \Big(\frac{1}{I_2} - \frac{1}{I_1}\Big) y_1 y_2 + \sum_{k=1}^{3} \Big(Q_{k1} \frac{\partial U(Q)}{\partial Q_{k2}} - Q_{k2} \frac{\partial U(Q)}{\partial Q_{k1}} \Big).$$

The Hamiltonian associated to (8) can be written as

$$H(y,Q) = \frac{1}{2}\Big(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\Big) + U(Q).$$

Recall that the Hamiltonian represents the mechanical energy of the system and that it is conserved along time.

Rigid body integrators

We first focus on numerical integrators for the free rigid body motion (4). We shall see further that such integrators can serve as basic brick to solve the rigid body equations (8) in the presence of external forces.

Quaternion implementation

For an efficient implementation, it is a standard approach to use quaternions to represent[2] the rotation matrices in $\mathbb{R}^3$, so that the multiplication of two rotations is equivalent to the product of the corresponding quaternions. Notice that the geometric properties of a rotation can be read directly on the corresponding quaternion. Precisely, any orthogonal matrix Q with $\det Q = 1$ can be represented by a quaternion q of norm $\|q\| = 1$ with $\|q\|^2 = q_0^2 + q_1^2 + q_2^2 + q_3^2$ by the relation

$$Q = \|q\|^2 I + 2q_0\widehat{e} + 2\widehat{e}^2, \qquad q = q_0 + iq_1 + iq_2 + kq_3,$$

[2] Other representations of rotations can be considered, in particular one can use the Euler angles (which may suffer from discontinuities) or one can also use simply 3×3 orthogonal matrices (usually more costly and subject to roundoff errors).

where the vector $e = (q_1, q_2, q_3)^T$ gives the axis of rotation in $\mathbb{R}^3$ and the rotation angle θ satisfies $\tan(\theta/2) = \sqrt{q_1^2 + q_2^2 + q_3^2}/q_0$. If Q is the orientation matrix of the rigid body, then the coefficients q_0, q_1, q_2, q_3 are called the Euler parameters of the rigid body.

Jacobi's analytic solution

$$\begin{aligned}
p &= -\frac{l}{A}\sin\vartheta\sin\varphi &&= -\sqrt{\frac{l^2 - Ch}{A(A-C)}}\cos\operatorname{am} u \\
q &= -\frac{l}{B}\sin\vartheta\cos\varphi &&= \sqrt{\frac{l^2 - Ch}{B(B-C)}}\sin\operatorname{am} u \\
r &= \frac{l}{C}\cos\vartheta &&= \pm\sqrt{\frac{Ah - l^2}{C(A-C)}}\,\Delta\operatorname{am} u,
\end{aligned}$$

Fig. 2. Facsimile of the free rigid body solution using Jacobi elliptic functions in the historical article of Jacobi (1850, p. 308). The constants A, B, C denote the moments of inertia.

Jacobi (1850) derived the analytic solution for the motion of a free rigid body and defined to this aim the so-called 'Jacobi analytic functions' as

$$\operatorname{sn}(u,k) = \sin(\varphi), \quad \operatorname{cn}(u,k) = \cos(\varphi), \quad \operatorname{dn}(u,k) = \sqrt{1 - k^2\sin^2(\varphi)}, \tag{9}$$

where the Jacobi amplitude $\varphi = \operatorname{am}(u,k)$ with modulus $0 < k \leq 1$ is defined implicitly by an elliptic integral of the first kind, see Jacobi's formulas in Figure 2. This approach can be used to design a numerical algorithm for the exact solution of the free rigid body motion. We refer to the article by Celledoni et al (2008) (see details on the implementation and references therein), and we mention that the Jacobi elliptic functions (9) can be evaluated numerically using the so-called arithmetic-geometric mean algorithm.

Algorithm 1 (Resolution of the Euler equations) *Assume $I_1 \leq I_2 \leq I_3$ (similar formulas hold for other orderings). Consider the constants*

$$c_1 = \frac{I_1(I_3 - I_2)}{I_2(I_3 - I_1)}, \qquad c_2 = 1 - c_1, \tag{10}$$

and the quantities

$$k_1 = \sqrt{y_1^2 + c_1 y_2^2}, \qquad k_2 = \sqrt{y_1^2/c_1 + y_2^2}, \qquad k_3 = \sqrt{c_2 y_2^2 + y_3^2}.$$

For $c_2 k_1^2 \le c_1 k_3^2$*, the solution of the Euler equations at time* $t = t_0 + h$ *is*[3]

$$y_1(t) = k_1 \operatorname{cn}(u,k), \quad y_2(t) = k_2 \operatorname{sn}(u,k), \quad y_3(t) = \delta k_3 \operatorname{dn}(u,k) = \delta\sqrt{k_3^2 - c_2 y_2(t)^2},$$

where we use the Jacobi elliptic functions (9) *with*

$$k^2 = \frac{c_2 k_1^2}{c_1 k_3^2}, \quad u = \delta h \lambda k_3 + \nu, \quad \lambda = \sqrt{\frac{(I_3 - I_2)(I_3 - I_1)}{I_1 I_2 I_3^2}},$$

$\delta = \operatorname{sign}(y_3) = \pm 1$*, and* ν *is a constant of integration determined from the initial condition* $y(t_0)$*. We have similar formulas for* $c_2 k_1^2 \ge c_1 k_3^2$*.*

The solution for the rotation matrix $Q(t)$ can next be obtained as follows. The angle $\theta(t)$ of rotation can be obtained by an elliptic integral of the third kind, the conservation of the angular momentum in the body frame yields $Q(t)y(t) = Q(t_0)y(t_0)$, which permits to recover the axis of the rotation $Q(t)$, see (Celledoni et al, 2008).

Splitting methods

Splitting methods are a convenient way to derive symplectic geometric integrators for the motion of a rigid body. This standard approach, proposed by McLachlan, Reich, and Touma and Wisdom in the 90', yields easy to implement explicit integrators. A systematic comparison of the accuracy of rigid body integrators based on splitting methods is presented by Fassò (2003). The main idea is to split the Hamiltonian $H(y)$ into several parts in such way that the equations can be easily solved exactly, using explicit analytic formulas (in most cases, the Euler equations shall reduce to the harmonic oscillator equations).

[3] Notice that k_1, k_2, k_3 are related to the square root terms in Fig. 2 and depend on y only via the conserved quantities $C(y), H(y)$. Here, we present a formulation different to Jacobi to avoid an unexpected roundoff error accumulation in the numerical implementation, see Vilmart (2008).

Three rotation splitting

One can consider the splitting

$$H(y) = R_1(y) + R_2(y) + R_3(y), \qquad \text{where } R_j(y) = y_j^2/(2I_j).$$

which yields the numerical method

$$\varphi_{h/2}^{R_3} \circ \varphi_{h/2}^{R_2} \circ \varphi_h^{R_1} \circ \varphi_{h/2}^{R_2} \circ \varphi_{h/2}^{R_1}$$

where $\varphi_h^{R_j}$ is the exact flow of (4) where in the matrix $J^{-1} = \mathrm{diag}(I_1^{-1}, I_2^{-1}, I_3^{-1})$, the values I_k^{-1} with $k \neq j$ are replaced by zero.

Symmetric+rotation splitting

It is often more efficient to consider the splitting given by the decomposition

$$H(y) = R(y) + S(y), \qquad \text{where } R(y) = \Big(\frac{1}{I_1} - \frac{1}{I_2}\Big)\frac{y_1^2}{2}, \quad S(y) = \frac{1}{2}\Big(\frac{y_1^2 + y_2^2}{I_2} + \frac{y_3^2}{I_3}\Big)$$

and defined by

$$\varphi_{h/2}^{R} \circ \varphi_h^{S} \circ \varphi_{h/2}^{R}.$$

Remark 3. Notice that this splitting method is exact if the rigid body is symmetric, i.e. for $I_1 = I_2$, but also for $I_1 = I_3$ or $I_2 = I_3$, and it is particularly advantageous in the case of a nearly symmetric body.

Consider for all scalar θ and vector $\omega = (\omega_1, \omega_2, \omega_3)^T$ the orthogonal matrices

$$U(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix}, \quad V(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \exp(\widehat{\omega}),$$

which can be respectively represented by the quaternions

$$u(\theta) = \cos(\theta/2) - i\sin(\theta/2), \qquad v(\theta) = \cos(\theta/2) - k\sin(\theta/2),$$

$$a(\omega) = \cos(\alpha/2) + \alpha^{-1}\sin(\alpha/2)(i\omega_1 + j\omega_2 + k\omega_3), \quad \alpha = \sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2},$$

where the formula for $a(\omega)$ is related to the Rodriguez formula for the exponential of a skew-symmetric matrix. Then, we have the following algorithm.

Algorithm 2 (Symmetric+Rotation splitting for the free rigid body motion)

1. *Apply the flow* φ_t^R *with* $t = h/2$ *given by*

$$y(t) = U(\alpha t)y(0), \qquad Q(t) = Q(0)U(-\alpha t), \qquad \alpha = y_1(0)/I_1.$$

2. *Apply the flow* φ_t^S *with* $t = h$ *given by*

$$y(t) = V(\beta t)y(0), \qquad Q(t) = Q(0)\exp(I_2^{-1}t\widehat{y(0)})V(-\beta t), \qquad \beta = I_3^{-1} - I_2^{-1}.$$

3. *Apply again the flow* φ_t^R *with* $t = h/2$.

RATTLE and the Discrete Moser-Veselov Algorithm

The RATTLE integrator is a famous symplectic numerical method for general constrained Hamiltonian systems. Applied to the rigid body problem (7), as proposed by McLachlan and Scovel, and Reich in the 90', it can be written as

$$\begin{aligned}
P_{1/2} &= P_0 - \frac{h}{2}\nabla U(Q_0) - \frac{h}{2}Q_0\Lambda_0 \\
Q_1 &= Q_0 + hP_{1/2}D^{-1}, \qquad Q_1^TQ_1 = I \\
P_1 &= P_{1/2} - \frac{h}{2}\nabla U(Q_1) - \frac{h}{2}Q_1\Lambda_1, \qquad Q_1^TP_1D^{-1} + D^{-1}P_1^TQ_1 = 0,
\end{aligned} \tag{11}$$

where Λ_0 and Λ_1 are symmetric matrices which can be eliminated using the constraints. Several approaches for the resolution of this system are discussed by McLachlan and Zanna (2005), (see also (14) below). The angular momentum y can be recovered from the matrices P, Q using $\hat{y} = Q^TP - P^TQ$. It can be checked that in the absence of an external potential ($U = 0$) this algorithm exactly conserves all quadratic invariants: the angular momentum in the body frame Qy, the Casimir $C(y)$, the Hamiltonian $H(y)$.

An integrable discretization of the free rigid body motion is the Discrete Moser–Veselov (DMV) algorithm Moser and Veselov (1991) with update for the orientation matrix proposed by Lewis and Simo (1996). It turns out that this discretisation is equivalent to the RATTLE algorithm applied to the free rigid body equations (see (11) with $U = 0$), as shown by McLachlan and Zanna (2005). The DMV algorithm can be formulated as

$$\widehat{y}_{n+1} = \Omega_n \, \widehat{y}_n \, \Omega_n^T, \qquad Q_{n+1} = Q_n \, \Omega_n^T, \tag{12}$$

where the orthogonal matrix Ω_n is computed from $\Omega_n^T D - D \, \Omega_n = h \, \widehat{y}_n$and $\Omega_n^T \Omega_n = I$. Some algebraic calculations yield the following quaternion implementation which is obtained by observing that the orthogonal matrix Ω_n^T in (12) can expressed thought the Caylay transform $\Omega_n^T = (I+\widehat{e}_n)(I+\widehat{e}_n)^{-1}$ where $e_n \in \mathbb{R}^3$ and Ω_n^T can be represented by a quaternion of norm 1,

$$\rho_n = \frac{1 + ie_{n,1} + je_{n,2} + ke_{n,3}}{\sqrt{1 + e_{n,1}^2 + e_{n,2}^2 + e_{n,3}^2}}. \tag{13}$$

Algorithm 3 *(Standard* DMV *algorithm for the free rigid body motion) Given the angular momentum y_n and the quaternion q_n corresponding to the orientation matrix Q_n at time t_0, we first compute compute the vector Y_n from the quadratic equation*

$$Y_n = \alpha_n y_n + \frac{h}{2} \widehat{Y}_n J^{-1} Y_n, \tag{14}$$

where $\alpha_n = 1 + e_{n,1}^2 + e_{n,2}^2 + e_{n,3}^2$ with $e_{n,j} = hY_{n,j}/(2I_j)$. This nonlinear system can be solved by using a few fixed-point iterations. The solution at time $t = t_0 + h$ is obtain by

$$y_{n+1} = y_n + \alpha_n^{-1} h \, \widehat{Y}_n J^{-1} Y_n, \qquad q_{n+1} = q_n \cdot \rho_n, \tag{15}$$

where the configuration update is given by a simple multiplication by the quaternion ρ_n given in (13) *with $e_{n,j} = hY_{n,j}/(2I_j)$.*

Remark 4. Suppressing the factor α_n in (14) and (15) yields the implicit midpoint rule for problem (4), which exactly conserves all first integrals of the system (in particular the orthogonality of Q) because these invariants are quadratic. Notice however that the

Table 1. Scalar functions for the preprocessed DMV algorithm (Alg. 4)

$$\delta = I_1 I_2 I_3, \qquad \sigma_a = I_1^a + I_2^a + I_3^a, \qquad \tau_{b,c} = \frac{I_2^b + I_3^b}{I_1^c} + \frac{I_3^b + I_1^b}{I_2^c} + \frac{I_1^b + I_2^b}{I_3^c},$$

$$\begin{aligned}
s_3(y) &= -\frac{\sigma_{-1}}{3} H(y) + \frac{\sigma_1}{6\delta} C(y), \qquad t_3(y) = \frac{\sigma_1}{6\delta} H(y) - \frac{1}{3\delta} C(y), \\
s_5(y) &= \frac{3\sigma_1 + 2\delta\sigma_{-2}}{60\delta} H(y)^2 + \frac{1 - \tau_{1,1}}{30\delta} C(y)H(y) + \frac{\sigma_2 - \delta\sigma_{-1}}{30\delta^2} C(y)^2, \\
t_5(y) &= -\frac{9 + \tau_{1,1}}{60\delta} H(y)^2 + \frac{6\delta\sigma_{-1} - \sigma_2}{60\delta^2} C(y)H(y) - \frac{\sigma_1}{60\delta^2} C(y)^2, \\
s_7(y) &= \frac{15 - \delta\sigma_{-3} - 2\tau_{1,1}}{630\delta} H(y)^3 + \frac{6\delta\tau_{1,2} - 100\delta\sigma_{-1} + 53\sigma_2}{2520\delta^2} C(y)H(y)^2 \\
&+ \frac{9\sigma_1 + 10\delta\sigma_{-2} - 6\tau_{2,1}}{420\delta^2} C(y)^2 H(y) + \frac{4\delta + 17\sigma_3 - 15\delta\tau_{1,1}}{2520\delta^3} C(y)^3, \\
t_7(y) &= \frac{9\delta\sigma_{-1} + \delta\tau_{1,2} - 11\sigma_2}{1260\delta^2} H(y)^3 + \frac{47\sigma_1 + 13\tau_{2,1} - 38\delta\sigma_{-2}}{2520\delta^2} C(y)H(y)^2 \\
&+ \frac{\sigma_3 + 2\delta\tau_{1,1} - 85\delta}{1260\delta^3} C(y)^2 H(y) + \frac{34\delta\sigma_{-1} - 19\sigma_2}{2520\delta^3} C(y)^3.
\end{aligned}$$

implicit midpoint rule *is not* a symplectic integrator for the constrained Hamiltonian system (7) formulated in the variables P, Q.

The RATTLE/DMV algorithm has only order two of accuracy. It is shown by Hairer and Vilmart (2006) that a suitable perturbation of the constant moments of inertia I_1, I_2, I_3 permits to improve the accuracy up to an arbitrarily high order of convergence, while sharing most of the geometric properties of the original DMV algorithm (see Table 2).

Algorithm 4 (Preprocessed DMV algorithm of high order $2p$ for the free rigid body)

1. *Compute the modified moments of inertia* $\widetilde{I}_j, j = 1, 2, 3$ *defined by*

$$\widetilde{I}_j^{-1} = I_j^{-1}\big(1 + h^2 s_3(y_n) + \ldots + h^2 s_{2p-1}(y_n)\big) + h^2 t_3(y_n) + \ldots + h^2 t_{2p-1}(y_n)$$

where the first scalar functions s_k, t_k *are given in Table 1 and depend on* y_n *only via the quadratic invariants* $C(y_n), H(y_n)$ *in* (5),(6).

2. *Apply the standard* DMV *algorithm (see Alg. 3) with the modified moments of inertia* $\widetilde{I}_j, j = 1, 2, 3$ *instead of the original ones.*

Rigid body integrators in the presence of an external potential

We now consider the case where the rigid body is subject to external forces. Consider the equations of motion of the rigid body (8) with an external potential $U(Q)$.

Example 1. (Heavy top) For instance, in the case of an asymmetric rigid body subject to gravity (heavy top), assuming that the third coordinate of the fixed frame is vertical and that the center of gravity of the rigid body has coordinates $(0,0,1)^T$ in the body frame, the potential energy due to gravity is given by $U(Q) = Q_{33}$.

Splitting method

A standard approach for the numerical treatment of an external force applied to the rigid body is to consider the usual Strang splitting method

$$\varphi^U_{h_2} \circ \Phi^T_h \circ \varphi^U_{h/2}, \tag{16}$$

or higher order splitting generalizations, or high-order compositions methods based on (16), where φ^U_t represents the exact flow of

$$\dot{Q} = 0, \qquad \dot{y} = -\operatorname{rot}(Q^T \nabla U(Q))$$

which can be expressed simply as $Q(t) = Q(0),\ y(t) = y(0) - t \operatorname{rot}(Q(0)^T \nabla U(Q(0)))$. Here, Φ^T_h is a suitable numerical method for the free rigid body problem (4) in the absence of an external potential, as presented previously.

High-order Nyström splitting methods

One can also consider standard high order splitting methods based on the flows Φ^T_h and Φ^U_h. It can be observed that the Poisson bracket $\{T, \{T, U\}\}$ vanishes, while the bracket $V = \{U, \{U, T\}\}$ is independent of y and depends only on the orientation matrix Q. This implies that classical Nyström splitting methods originally designed for solving order two differential equations can successfully be applied in our context.

These methods involve not only the flows associated to the Hamiltonian $T(y)$ and the potential $U(Q)$, but also the potential $V(Q)$. For instance, one can use the splitting method

$$\varphi^U_{h/6} \circ \varphi^T_{h/2} \circ \varphi^U_{2h/3} \circ \varphi^V_{-h^3/72} \circ \varphi^T_{h/2} \circ \varphi^U_{h/6}$$

which is a symmetric scheme of order 4, or other higher order generalizations as studied by Blanes et al (2001). Notice that in the case of the heavy top (Example 1) where $U(Q) = Q_{33}$, the flows φ^U_h, φ^V_h are the exact solutions of $\dot{Q} = 0,\ \dot{y} = (Q_{32}, -Q_{31}, 0)^T$, and $\dot{Q} = 0,\ \dot{y} = (Q_{32}Q_{33}/I_1, -Q_{31}Q_{33}/I_2, 0)^T$, respectively.

Comparison of the geometric properties of the free rigid body integrators

Table 2. Geometric properties of free rigid body integrators

integrator	order of accuracy	exact preservation of quadratic invariants			Poisson	symplectic
		Qy	$C(y)$	$H(y)$		
Jacobi's analytic solution (see Alg. 1)	exact	√	√	√	√	√
Symmetric+Rotation splitting (Alg. 2)	2	√	√	no	√	√
RATTLE/DMV algorithm (Alg. 3)	2	√	√	√	√	√
Implicit midpoint rule (Rem. 4)	2	√	√	√	no	no
Preprocessed DMV algorithm (Alg. 4)	$2p$	√	√	√	√	no

We compare in Table 2 the geometric properties of the free rigid body integrators presented in this entry. Column "symplectic" indicates whether the method is a symplectic integrator. In the context of backward error analysis this means that the numerical solution y_n, Q_n formally coincides with the exact solution at time $t_n = nh$ of the modified differential equation, which is of the form

$$\dot{y} = \widehat{y}\,\nabla \widetilde{H}_h(y), \qquad \dot{Q} = Q\,\widehat{\nabla \widetilde{H}_h(y)},$$

where $\widetilde{H}_h = H + hK_2 + \dots$ is a formal series in powers of h. If it has this form only for the y component, the method is still a Poisson integrator (column "Poisson").

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