

The discrete Moser–Veselov algorithm for the free rigid body

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Overview

The subject of this talk is the numerical solution of the free RB equations,

$$M' = [M, \Omega], \quad M = \Omega J + J \Omega,$$

where M, Ω are skew-symmetric matrices and J is a diagonal matrix with positive entries.

M is the matrix of **body momenta**

Ω is the matrix of **body angular velocity**

Often the above equations are associated with the equations that give the configuration of the body in the fixed frame,

$$Q' = Q\Omega, \quad Q \in \text{SO}(N).$$

- The Discrete Moser–Veselov description of the rigid body
- Integrability of the discrete algorithm
- Backward error analysis of the the DMV algorithm
- Higher order integrable approximations
- Numerical experiments and comparisons with other methods
- Explicit methods for the 3×3 case



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The Moser–Veselov discrete version of the dynamics of a Rigid Body

The Lagrangian of the continuous RB equations, is the kinetic energy,

$$L = \frac{1}{2} \text{tr}(\Omega^\top M) = \frac{1}{2} \text{tr}(-\Omega^2 J - \Omega J \Omega) = \text{tr}(\Omega^\top J \Omega), \quad (1)$$

where we take into account that $\Omega^\top = -\Omega$ and that the trace is invariant under cyclic permutations. Following (Marsden, Pekarsky & Shkoller 1999), discretise $\Omega = X^{-1} \dot{X}$, where $X \in \text{SO}(N)$ is the configuration of the body, using a finite difference approximation of the derivative,

$$\Omega = X^{-1} \dot{X} \approx \frac{1}{h} X_{k+1}^\top (X_{k+1} - X_k), \quad X_k, X_{k+1} \in \text{SO}(N),$$

which gives

$$L \approx \frac{1}{h^2} \text{tr}(J - X_k^\top X_{k+1} J - J X_{k+1}^\top X_k - X_k^\top X_{k+1} J X_{k+1}^\top X_k).$$

Due to the orthogonality of the X_k 's and the cyclicity of the trace, the first and the last term cancel, and moreover, we can write

$$L \approx \frac{2}{h^2} \text{tr}(X_k J X_{k+1}^\top).$$

Up a scaling factor, this is precisely the discrete Lagrangian of Moser and Veselov.



Consider the functional $S(X)$ determined by

$$S = \sum_k \text{tr}(X_k J X_{k+1}^\top)$$

where $X = \{X_k\}$ with $X_k \in O(N)$ and J is a diagonal matrix. To obtain the stationary points of S , we consider

$$\sum_k \text{tr}(X_k J X_{k+1}^\top) - \frac{1}{2} \sum_k \text{tr}(\Lambda_k (X_k X_k^\top - I)),$$

(where $\Lambda_k = \Lambda_k^\top$ is a Lagrange multiplier), and $\delta S = 0$ becomes

$$X_{k+1} J + X_{k-1} J = \Lambda_k X_k,$$

from which, multiplying by X_k^\top on the right and taking into consideration the symmetry of Λ_k ,

$$X_{k+1} J X_k^\top + X_{k-1} J X_k^\top = \Lambda_k = \Lambda_k^\top = X_k J X_{k+1}^\top + X_k J X_{k-1}^\top, \quad (2)$$

hence, the *discrete analogue of the angular momentum in space*,

$$m_k = X_k J X_{k-1}^\top - X_{k-1} J X_k^\top,$$

is conserved.



In the body variables, setting $\omega_k = X_k^\top X_{k-1} \in O(N)$ and $M_k = X_{k-1}^{-1} m_k X_{k-1} = \omega_k^\top J - J \omega_k \in \mathfrak{so}(N)^*$ (angular momentum w.r.t. the body), (2) becomes

$$\begin{aligned} M_{k+1} &= \omega_k M_k \omega_k^\top \\ M_k &= \omega_k^\top J - J \omega_k. \end{aligned} \tag{3}$$

the **discrete Euler–Arnold** equation.

In the continuous limit: when $t_k = t_0 + k\varepsilon$, $k = 0, 1, 2, \dots$,

- $X_k = X(t_k)$
- $\omega_k = X_k^\top X_{k-1} \approx I - \varepsilon \Omega(t_k)$,
- $M_k \approx \varepsilon(J\Omega + \Omega J) = \varepsilon M(t_k)$,

letting $\varepsilon \rightarrow 0$, one obtains the familiar Euler–Arnold equations for the motions of the N -dimensional rigid body,

$$\begin{aligned} M' &= [M, \Omega] \\ M &= J\Omega + \Omega J, \quad \Omega \in \mathfrak{so}(N). \end{aligned}$$





To solve the discrete Euler–Arnold equations (3):

- For $k = 0, 1, 2, \dots$, find $\omega_k \in \text{SO}(N)$ such that $M_k = \omega_k^\top J - J\omega_k$.
- Update $M_{k+1} = \omega_k M_k \omega_k^\top$.

By construction, this algorithm

- preserves exactly momentum and energy (integrable map)
- is a second order approximation to the continuous rigid body
- preserves the standard Poisson structure of $T^*\mathfrak{so}(N)$,

$$\{f, g\} = \text{tr}(M[f_M, g_M]), \quad f, g \in C^\infty(\mathfrak{so}(N)),$$

where $f_M = (\partial f / \partial M_{i,j})$.

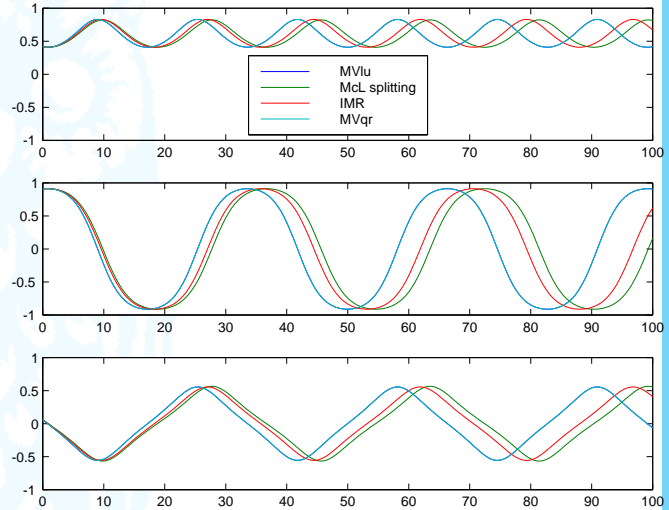
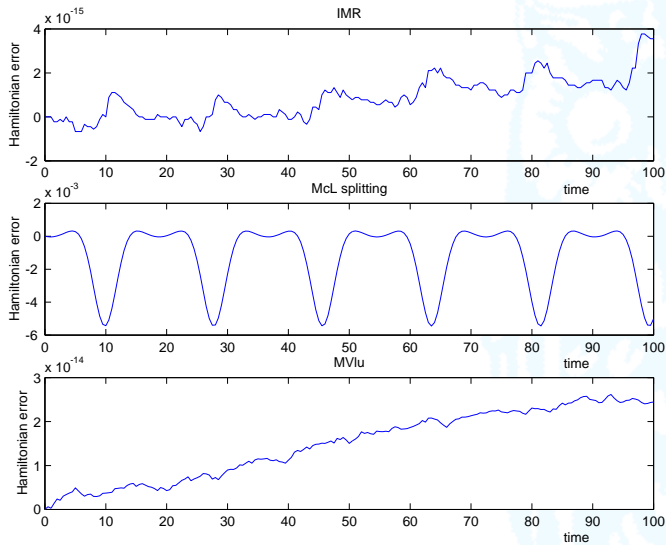
Note that

- Also the IMR is second order, preserves all the integrals of the continuous rigid body.
- Another much used method is a Lie–Poisson integrator of McLachlan and Reich (LP2). For the 3×3 RB, it consists in splitting the Hamiltonian

$$H = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3 = \frac{m_1^2}{J_2 + J_3} + \frac{m_2^2}{J_1 + J_3} + \frac{m_3^2}{J_1 + J_2}$$

and integrating explicitly (a la Strang) the vector fields of each split Hamiltonian. The method is second order, explicit, preserves the Poisson structure but does not preserve H .





Error in the Hamiltonian function H in the interval $[0, 100]$ and for $h = \frac{1}{2}$.

The components of the vector \mathbf{m}_k for $h = \frac{1}{2} \dots$

$$\mathbf{m} = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \equiv \hat{\mathbf{m}} = M = \begin{bmatrix} 0 & -m_3 & m_2 \\ m_3 & 0 & -m_1 \\ -m_2 & m_1 & 0 \end{bmatrix}$$



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Integrability of the Moser–Veselov equation

Recall the Moser–Veselov equation,

$$M_k = \omega_k^\top J - J\omega_k, \quad M_k^\top = -M_k, \quad \omega_k^\top \omega_k = I. \quad (4)$$

in tandem with the update $M_{k+1} = \omega_k M_k \omega_k^\top$.

- The Moser–Veselov equation (4) has not a unique solution;

Lemma 1 (*Moser and Veselov*) Equation (4) is equivalent to the factorization

$$(I - \lambda M_k - \lambda^2 J^2) = (\omega_k^\top + \lambda J)(\omega_k - \lambda J)$$

Rewrite the above factorization as

$$(I - \lambda M_k - \lambda^2 J^2) = A_k^\top(\lambda) A_k(\lambda) \quad A_k(\lambda) = (\omega_k - \lambda J)$$

and define the mapping with image point M_{k+1} such that

$$(I - \lambda M_{k+1} - \lambda^2 J^2) = A_k(\lambda) A_k^\top(\lambda).$$

By construction,

$$(I - \lambda M_{k+1} - \lambda^2 J^2) = A_k(\lambda)(I - \lambda M_k - \lambda^2 J^2)A_k^{-1}(\lambda),$$

hence the map is an **integrable** as it is an isospectral flow.



BEA for DMV

Recall the DMV equations and the continuous RB equations

$$\begin{aligned}M_{k+1} &= \omega_k M_k \omega_k^\top, & M' &= [M, \Omega] \\M_k &= \omega_k^\top J - J \omega_k, & M &= \Omega J + J \Omega,\end{aligned}$$

where $\omega_k \approx I - h\Omega(t_k)$.

We wish to write

$$M_{k+1} = \Phi_h(M_k) = M_k + h[M_k, \Omega_k] + h^2 d_2 + h^3 d_3 + h^4 d_4 + \dots,$$

and find the modified vector field

$$\tilde{M}' = [\tilde{M}, \tilde{\Omega}] + h f_2(\tilde{M}, \tilde{\Omega}) + h^2 f_3(\tilde{M}, \tilde{\Omega}) + h^3 f_4(\tilde{M}, \tilde{\Omega}) + \dots \quad (5)$$

such that $\Phi_h(M_k)$ equals the solution $\tilde{M}(t_{k+1})$ at time $t_{k+1} = t_0 + (k+1)h$ of the modified vector field (5).

To find $\Phi_k(h)$, we write

$$\omega_k = \exp(-h\Omega_0 - h^2\Omega_1 - h^3\Omega_2 - h^4\Omega_3 - h^5\Omega_4 + \dots), \quad (6)$$

where $\Omega_0, \Omega_1, \Omega_2, \dots$, are skew-symmetric matrices computed so that

$$\omega_k^\top J - J \omega_k = h(\Omega(t_k)J + J\Omega(t_k)). \quad (7)$$



we obtain

$$\begin{aligned} h(\Omega(t_k)J + J\Omega(t_k)) &= h(\Omega_0J + J\Omega_0) + h^2(\Omega_1J + J\Omega_1 + \frac{1}{2}(\Omega_0^2J - J\Omega_0^2)) \\ &\quad + h^3(\Omega_2J + J\Omega_2 + \frac{1}{2}[(\Omega_0\Omega_1 + \Omega_1\Omega_0), J] + \frac{1}{6}(\Omega_0^3J + J\Omega_0^3)) + \dots \end{aligned}$$

Comparing left and right-hand-sides, it is trivially observed that the order- h term disappears if $\Omega_0 = \Omega$ (to simplify notation, we omit the dependence of Ω on t_k). In order to annihilate the h^2 -term, we require that

$$\Omega_1J + J\Omega_1 + \frac{1}{2}(\Omega_0^2J - J\Omega_0^2) = 0.$$

Recall that $M = \Omega J + J\Omega$ and hence $M' = \Omega'J + J\Omega'$. On the other hand, $M' = [M, \Omega] = -(\Omega^2J - J\Omega^2)$. Hence we can write

$$O = \Omega_1J + J\Omega_1 - \frac{1}{2}M' = \Omega_1J + J\Omega_1 - \frac{1}{2}(\Omega'J + J\Omega')$$

and the identity is satisfied by if and only if

$$\Omega_1 = \frac{1}{2}\Omega'. \quad (8)$$

In general, the **algorithm** to derive Ω_i , for $i = 1, 2, \dots$, is

1. Find the coefficient of h^{i+1} in (7) and set it equal to zero. This will give an equation of the type $\Omega_iJ + J\Omega_i = C_iJ + JC_i + [D_i, J]$. Note that the terms $C_iJ + JC_i$ have an odd occurrence of the Ω_j s, while the terms of the type $[D_i, J]$ have an even occurrence of the Ω_j s.
2. Use the derivatives of M and Ω to express the term $[D_i, J]$ as $\tilde{C}_iJ + J\tilde{C}_i$.



3. Deduce $\Omega_i = C_i + \tilde{C}_i$.

$$\begin{aligned}\Omega_0 &= \Omega \\ \Omega_1 &= \frac{1}{2}\Omega' \\ \Omega_2 &= \frac{1}{6}\Omega'' - \frac{1}{6}\Omega^3 \\ \Omega_3 &= \frac{1}{8}\Omega''' - \frac{1}{24}(5\Omega^2\Omega' + 2\Omega\Omega'\Omega + 5\Omega'\Omega^2)\end{aligned}$$

The functions Ω_i

Once the Ω_i s are known, substituting back in $M_{k+1} = \omega_k^\top M_k \omega_k$ and using the well known identity

$$\exp(X)Y \exp(-X) = \exp_{\text{ad}_X} Y = \sum_{k=0}^{\infty} \frac{1}{k!} \text{ad}_X^k(Y),$$

where $\text{ad}_X(Y) = [X, Y]$ and, recursively, $\text{ad}_X^k(Y) = [X, \text{ad}_X^{k-1}(Y)]$, we find the expressions for the functions d_i in terms of the $\Omega_{i-1}, \Omega_{i-2}, \dots, \Omega_0$,

$$d_i = \sum_{j=1}^i \frac{(-1)^j}{j!} \sum_{k_1+k_2+\dots+k_j=i-j} \text{ad}_{\Omega_{k_1}} \text{ad}_{\Omega_{k_2}} \cdots \text{ad}_{\Omega_{k_j}} M, \quad k_1, \dots, k_j \in \{0, 1, \dots, i-1\}. \quad (9)$$

$$\begin{aligned}d_2 &= \frac{1}{2}([M, \Omega'] + [[M, \Omega], \Omega]), \\ d_3 &= \frac{1}{4}[M, \Omega''] + \frac{1}{4}[[M, \Omega'], \Omega] + \frac{1}{4}[[M, \Omega], \Omega'] + \frac{1}{6}[[[M, \Omega], \Omega], \Omega] - \frac{1}{6}[M, \Omega^3], \\ d_4 &= \dots,\end{aligned} \quad (10)$$

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Taylor expansion of the solution of the modified equation

Consider

$$\frac{d}{dt}\tilde{y} = f(\tilde{y}) + hf_2(\tilde{y}) + h^2f_3(\tilde{y}) + \dots,$$

where $f(M) = [M, \Omega] = [M, \mathcal{J}^{-1}M]$ is the original vector field of the RB equations, where \mathcal{J} is a linear operator, defined such that $\mathcal{J}\Omega = \Omega\mathcal{J} + \mathcal{J}\Omega = M$. Putting $\tilde{y}(t) = M(t)$, we expand the solution of the above equation in a Taylor series and collect corresponding powers of h ,

$$\begin{aligned}\tilde{y}(t+h) &= M(t) + hf(M) + h^2 \left(f_2(M) + \frac{1}{2!}f'f(M) \right) \\ &\quad + h^3 \left(f_3(M) + \frac{1}{2!}(f'f_2(M) + f_2'f(M)) + \frac{1}{3!}(f''(f, f)(M) + f'f'f(M)) \right) + \dots,\end{aligned}$$

where f' is considered as a linear operator, f'' as a bilinear operator and so on and so forth. In our case,

$$\begin{aligned}f'(z)(M) &= [z, \mathcal{J}^{-1}M] + [M, \mathcal{J}^{-1}z] \\ &= [z, \Omega] + [M, \mathcal{J}^{-1}z] \\ f''(z_1, z_2)(M) &= 2[z_1, \mathcal{J}^{-1}z_2],\end{aligned}$$

and, since f is quadratic, f''' and all the other higher derivatives equal zero.

At this point it is important to stress an important difference between the expressions for the modified vector field of (Hairer, Lubich & Wanner 2002) and ours. While the vector field discussed in (Hairer et al. 2002) is in \mathbb{R}^n , hence the f'' is a symmetric quadratic operator, this is not the case for our vector field which is on matrices, thus

$$f''(f'f, f) \neq f''(f, f'f).$$

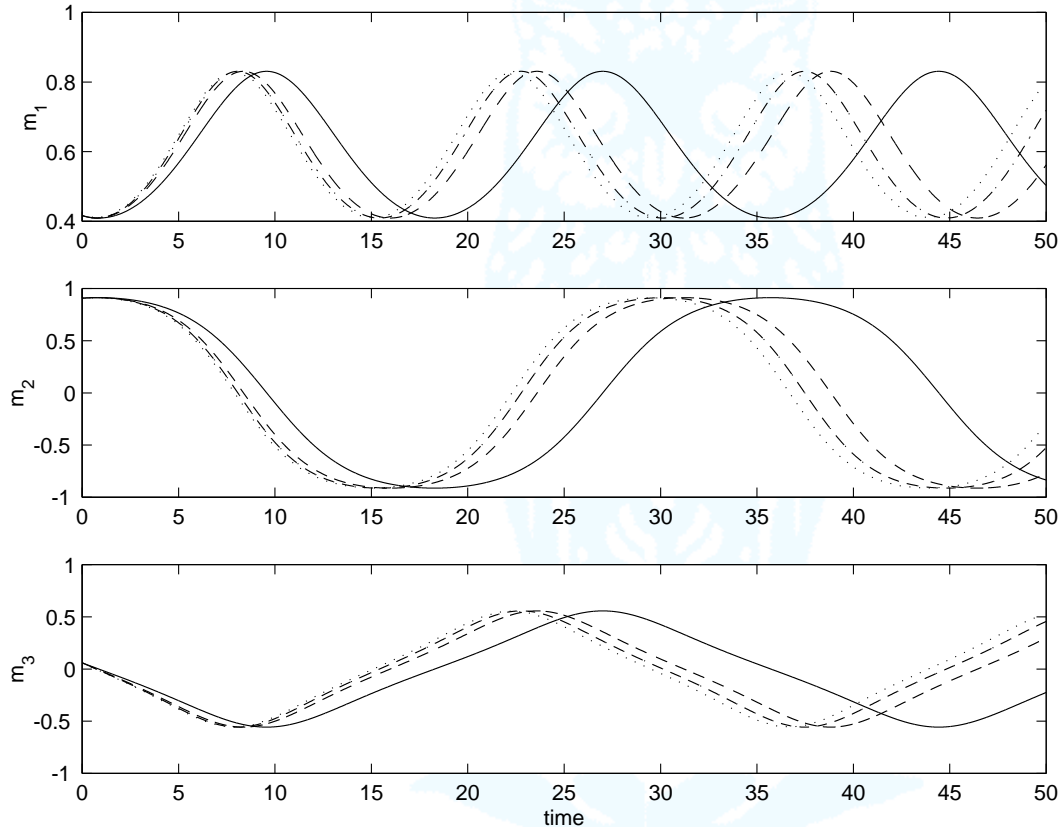


This non-commutative case is discussed with more generality in (Munthe-Kaas & Krogstad 2002). However, we observe that *all* the terms containing combinations of f'' , f' and f correspond simply to higher derivatives of f . The mixed terms are treated instead specifically.

After some algebra, we have

$$\begin{aligned}
 f_2 &= d_2 - \frac{1}{2!} f' f(M) \\
 &= O, \\
 f_3 &= d_3 - \frac{1}{3!} (f''(f, f)(M) + f' f' f(M)) \\
 &= \frac{1}{12} [M, \Omega'' - [\Omega, \Omega'] - 2\Omega^3], \\
 f_4 &= d_4 - \frac{1}{4!} M^{(iv)} - \frac{1}{2!} (f' f_3 + f_3' f) \\
 &= O, \\
 f_5 &= d_5 - \frac{1}{5!} M^{(v)} - \frac{1}{2!} (f' f_4 + f_4' f' + \frac{1}{2!} \frac{d}{dt} (f_3' f + f' f_3)) \\
 &= \frac{1}{80} [M, \Omega^{(iv)}] - \frac{1}{80} [M, [\Omega, \Omega''']] + \frac{3}{40} [M, \Omega^5 - \Omega' \Omega \Omega'] \\
 &\quad + \frac{1}{80} [M, [\Omega', \Omega'']] - \frac{1}{40} [M, \Omega \Omega'' \Omega] - \frac{1}{20} [M, \Omega^2 \Omega'' + \Omega'' \Omega^2] \\
 &\quad + \frac{1}{20} [M, [\Omega^3, \Omega']] - \frac{1}{40} [M, \Omega \Omega'^2 \Omega + \Omega \Omega \Omega'^2 + \Omega [\Omega, \Omega'] \Omega].
 \end{aligned} \tag{11}$$





The DMV solution of the RB equations (dotted line), the exact solution (solid line) and the trajectories corresponding to the modified vector fields $f + h^2 f_3$ (dashed line) and $f + h^2 f_3 + h^4 f_5$ (dash-dotted line) in the interval $[0, 50]$ with $h = \frac{8}{10}$.



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Some important results about DMV

Theorem 2 *The DMV is time-reversible, hence $f_{2i} = 0$, $i = 1, 2, \dots$*

Theorem 3 (Moser–Veselov) *In the 3×3 case, the DMV is a time-reparametrisation of the flow of the original vector field of the rigid body.*

Since the mapping preserves the underlying Poisson structure and all the integrals $F_i = c_i$ of the system, it commutes with all commuting Hamiltonian flows generated by the F_i s, $M' = \{M, \nabla F_i\}$. The nonsingular compact level sets $T_c = \cap_i (F_i = c_i)$ consists of a finite union of 1-dimensional tori and on each torus the DMV mapping is a shift along the trajectory depending on the integral quantity H_2 .

Hence, the DMV solves the modified equation

$$M' = (1 + h^2\tau_3 + h^4\tau_5 + \dots + h^{2i}\tau_{2i+1} + \dots)[M, \Omega],$$

where h is the stepsize of integration and the τ_{2i+1} , for $i = 1, 2, \dots$, are constants.



Introduce the constants

$$\begin{aligned}C_{J,i,j} &= J_1^i J_2^j + J_1^i J_3^j + J_2^i J_3^j, \\C_{J,i} &= C_{J,i,i} \\C_J &= C_{J,1} \\ \Delta &= (J_1 + J_2)(J_1 + J_3)(J_2 + J_3) \\ H_2 &= (J_1 + J_2)(J_1 + J_3)(J_2 + J_3)H - C_J \|\mathbf{m}\|_2.\end{aligned}$$

Theorem 4 *One has*

$$\tau_3 = \frac{1}{6\Delta^2}((3 \det(J)\text{tr}(J) + C_{J,2})\|\mathbf{m}\|_2^2 + (3C_J + \text{tr}(J^2))H_2),$$

and

$$\begin{aligned}\tau_5 &= \frac{1}{40\Delta^4} \left((3\text{tr}(J^4) + 27C_{J,2} + 15\text{tr}(J^2)C_J + 45 \det(J)\text{tr}(J))H_2^2 \right. \\ &\quad + (10C_{J,3} + 50 \det(J)\text{tr}(J)C_J + 10 \det(J)\text{tr}(J)\text{tr}(J^2) + 2C_{J,2}\text{tr}(J^2) - 28 \det(J^2))\|\mathbf{m}\|_2^2 H_2 \\ &\quad \left. + (60 \det(J^2)C_J + 3C_{J,4} + 27 \det(J^2)\text{tr}(J^2) + 15 \det(J)(C_{J,2,3} + C_{J,3,2}))\|\mathbf{m}\|_2^4 \right).\end{aligned}$$

Proof. By direct computation of f_3 and f_5 . □





Higher-order integrable methods

For the original RB equations, scaling the initial condition is equivalent to scaling time.

In our case, we know that DMV is a time-rescaling of the original RB equation. Therefore we wish to rescale the initial condition to obtain a better approximation of the unscaled original RB.

I.C. DMV

New I.C. DMV

$$h(\Omega(t_k)J + J\Omega(t_k)) \quad \frac{h(\Omega(t_k)J + J\Omega(t_k))}{1 + \tilde{\tau}_3 h^2 + \tilde{\tau}_5 h^4 + \dots}$$

We perform again the backward error analysis. We set now $\tilde{\omega} = \exp(-h\tilde{\Omega}_0 - h^2\tilde{\Omega}_1 + \dots)$ and solve for the $\tilde{\Omega}_i$ s as the skew-symmetric matrices that solve

$$h(1 - \tilde{\tau}_3 h^2 + (\tilde{\tau}_3^2 - \tilde{\tau}_5)h^4 + \dots)(\Omega J + J\Omega) = \tilde{\omega}^\top J - J\tilde{\omega}. \quad (12)$$

$$\begin{aligned} \tilde{f}_3 &= \tilde{d}_3 - \frac{1}{3!}M''' = -\tilde{\tau}_3[M, \Omega] + d_3 - \frac{1}{3!}M''' \\ &= -\tilde{\tau}_3[M, \Omega] + f_3 = (-\tilde{\tau}_3 + \tau_3)[M, \Omega], \end{aligned}$$

hence, in order to have an order-four scheme, we must set $\tilde{f}_3 = 0$ which corresponds to the choice

$$\tilde{\tau}_3 = \tau_3.$$



After further computations, one has

$$\tilde{f}_5 = 0 \leftrightarrow \tilde{\tau}_5 = \tau_5 - 2\tau_3^2.$$

This value of $\tilde{\tau}_5$ gives indeed a method of order six.

The new proposed algorithms of order four and six are described below.

The DMV4 algorithm:

1. Compute τ_3 and set $M_0 := M(t_0)h/(1 + h^2\tau_3)$.
2. For $k = 0, 1, \dots, n - 1$,
find the unique w_k as above such that $M_k = \omega_k^\top J - J\omega_k$
set $M_{k+1} = \omega_k M_k \omega_k^\top$
end
3. Reconstruct $M_n := M_n(1 + h^2\tau_3)/h \approx M(t_n)$.

The DMV6 algorithm:

1. Compute τ_3, τ_5 and set $\tilde{\tau}_5 = \tau_5 - 2\tau_3^2$ and $M_0 := M(t_0)h/(1 + h^2\tau_3 + h^4\tilde{\tau}_5)$.
2. For $k = 0, 1, \dots, n - 1$,
find the unique w_k as above such that $M_k = \omega_k^\top J - J\omega_k$
set $M_{k+1} = \omega_k M_k \omega_k^\top$
end
3. Reconstruct $M_n := M_n(1 + h^2\tau_3 + h^4\tilde{\tau}_5)/h \approx M(t_n)$.



Some numerical experiments

We consider with initial condition

$$\mathbf{m}_0 = \begin{bmatrix} 0.4165 \\ 0.9072 \\ 0.0588 \end{bmatrix}$$

and matrix J given as

$$J = \begin{bmatrix} 0.9218 & 0 & 0 \\ 0 & 0.7382 & 0 \\ 0 & 0 & 0.1763 \end{bmatrix}$$

and compare the DMV explicit scheme with the Hamiltonian-splitting method LP2 of (McLachlan 1993)

$$H = \frac{m_1^2}{J_2 + J_3} + \frac{m_2^2}{J_1 + J_3} + \frac{m_3^2}{J_1 + J_2} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3$$

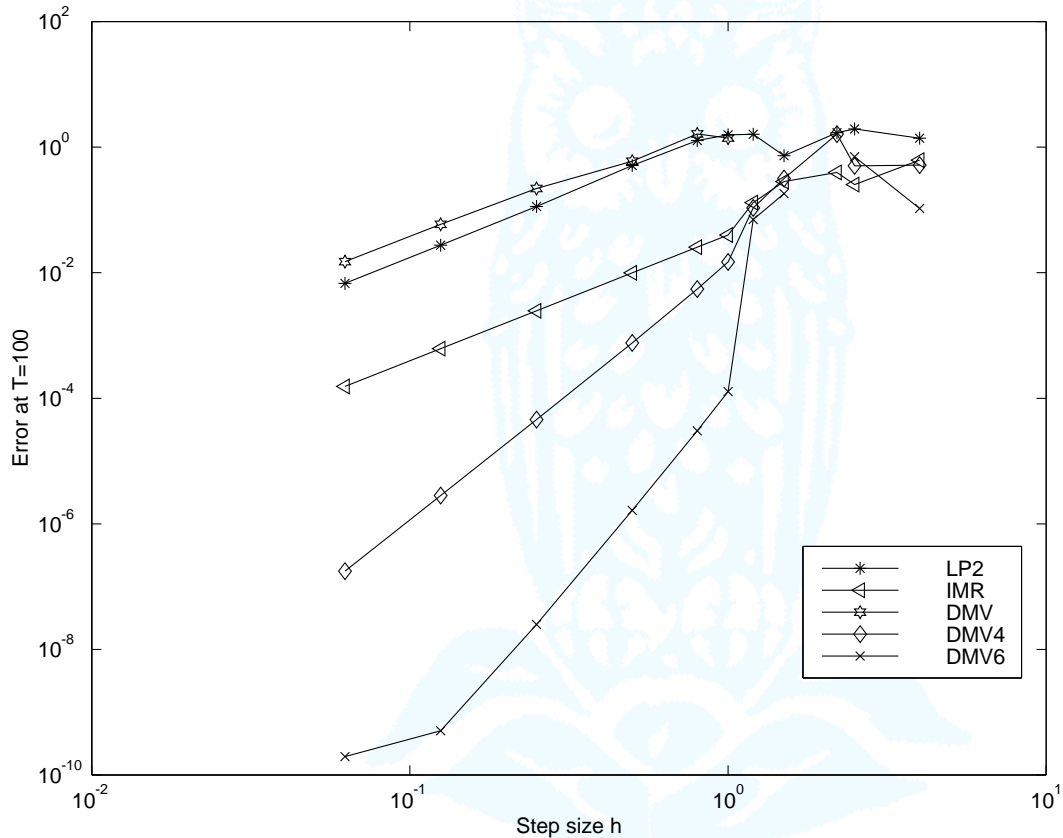
and the Implicit Midpoint Rule (IMR),

$$\mathbf{m}_{k+1} = \mathbf{m}_k + hf\left(\frac{\mathbf{m}_k + \mathbf{m}_{k+1}}{2}\right),$$

where

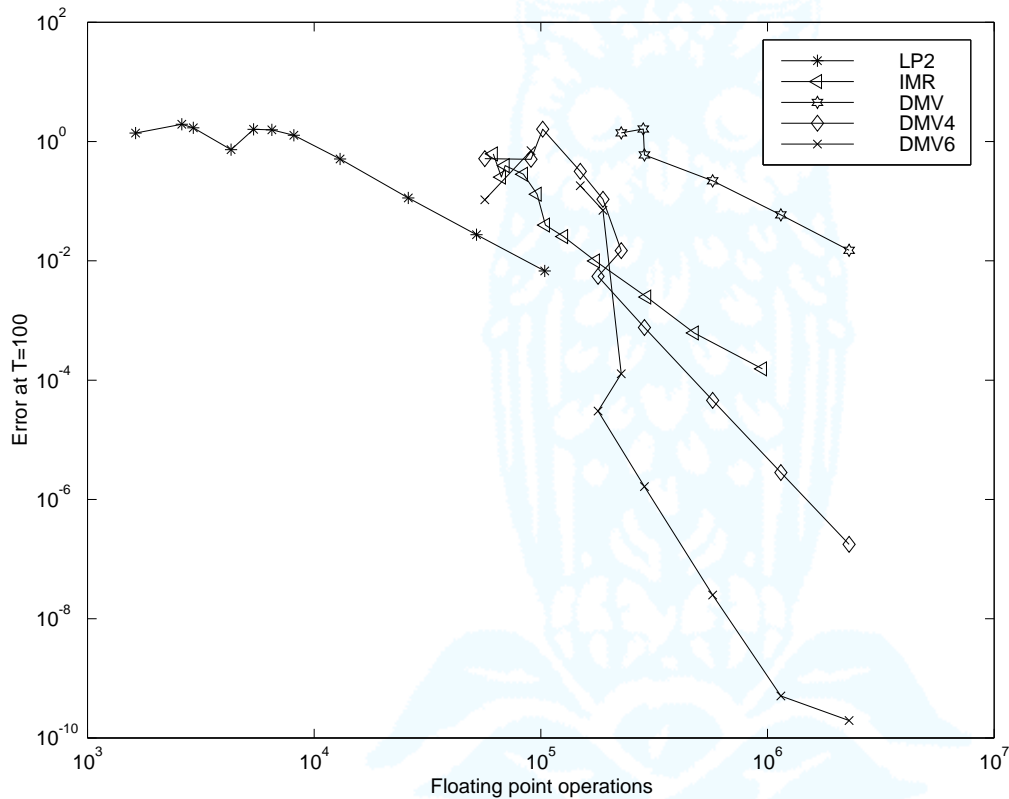
$$\mathbf{f}(\mathbf{m}) = \mathbf{m} \times (\tilde{J})^{-1} \mathbf{m}, \quad \tilde{J} = \begin{bmatrix} J_2 + J_3 & 0 & 0 \\ 0 & J_1 + J_3 & 0 \\ 0 & 0 & J_1 + J_2 \end{bmatrix}.$$





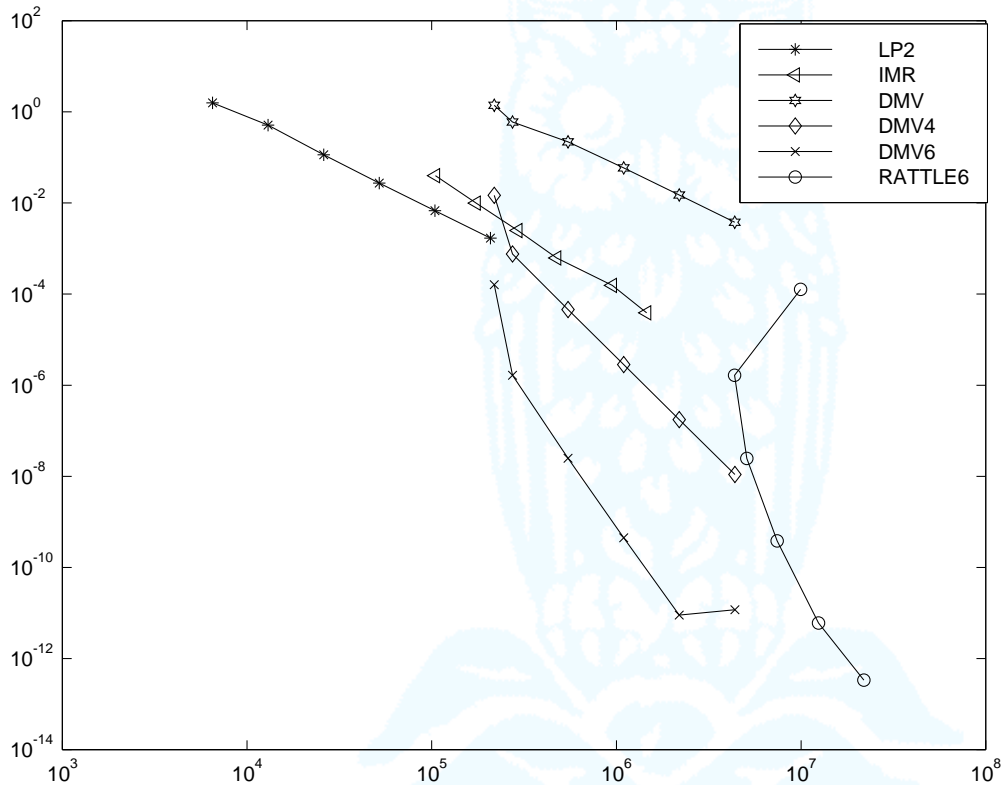
Error versus step size computed at $T = 100$ for the methods LP2, IMR, DMV, DMV4, DMV6.





Floating point operations versus accuracy ($T = 100$) for the methods LP2, IMR, DMV, DMV4, DMV6. The roots of $P(\lambda)$ are recomputed at each step, use QR with pivoting, (DMV ≈ 22 LP2 per step).





Floating point operations versus accuracy ($T = 100$) for the methods LP2, IMR, DMV, DMV4, DMV6 and RATTLE6. The roots of $P(\lambda)$ are computed once, use LU instead of QR (DMV ≈ 19)



Back

Close

LP2 per step).

Method	$h = \frac{1}{16}$	$h = \frac{1}{2}$	$h = 1.2$	$h = 2.2$	$h = 2.5$	$h = 4$
LP2	6.7903e-03	5.1043e-01	1.6055e+00	1.7002e+00	1.9489e+00	1.3902e+00
IMR	1.5494e-04	9.9329e-03	1.3119e-01	3.9514e-01	2.5276e-01	6.1905e-01
DMV	1.5014e-02	5.9899e-01	NaN	NaN	NaN	NaN
DMV4	1.757e-07	7.6167e-04	1.0785e-01	1.6094e+00	5.0245e-01	5.1624e-01
DMV6	1.962e-10	1.6440e-06	7.0269e-02	NaN	7.0407e-01	1.0519e-01

Error for the various methods and selected step sizes



Connections with matrix Riccati equations

Consider the matrix equation

$$M = XJ - JX^\top. \quad (13)$$

Cardoso & Leite (2003) shown that every solution of (13) (not necessarily orthogonal) is of the form

$$X = (M/2 + S)J^{-1},$$

for some symmetric matrix S .

Furthermore, X is a *orthogonal* solution of (13) if and only if S is a symmetric solution of the Riccati equation

$$S^2 + S(M/2) + (M/2)^\top S - (M^2/4 + J^2) = 0. \quad (14)$$

Riccati equations are associated to symplectic matrices. In our case, the symplectic matrix is

$$H_{\text{symp}} = \begin{bmatrix} \frac{M}{2} & I \\ \frac{M^2}{4} + J^2 & \frac{M}{2} \end{bmatrix}. \quad (15)$$

If $\frac{M^2}{4} + J^2$ is positive definite, it has been shown in (Cardoso & Leite 2003) that (14) has a unique solution S which is symmetric, positive definite, and such that the eigenvalues of $W = M/2 + S$ have positive real parts. This matrix W is precisely the same matrix in Moser & Veselov (1991), from which one obtains

$$\omega = WJ^{-1}.$$



Algorithm(Cardoso & Leite 2003): Compute X , the unique solution of (13) in the special orthogonal group $SO(n)$.

1. Find a real Schur form of H_{symp1} ,

$$\tilde{Q}^\top H_{\text{symp1}} \tilde{Q} = \begin{bmatrix} T_{11} & T_{12} \\ O & T_{22} \end{bmatrix}, \quad (16)$$

where T_{11} and T_{22} are block upper-triangular matrices such that the real parts of the spectrum of T_{11} are positive and the real parts of the spectrum of T_{22} are negative definite.

2. Partition \tilde{Q} accordingly,

$$\tilde{Q} = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}.$$

Then, compute

$$S = Q_{21} Q_{11}^{-1}.$$

3. Compute

$$X = \left(\frac{M}{2} + S \right) J^{-1}.$$

Some computational details

- Compute real Schur forms by QR iterations for eigenvalues (Golub & van Loan 1989)
- Cost: $\mathcal{O}((2N)^3)$ operations (implicit methods for ODEs: $\mathcal{O}(N^3)$)

N being the dimension of M .





The case $N = 3$

In this case,

- it is possible to find an **explicit spectral decomposition** of H_{symp1} (without the QR eigenvalue method)
- construct the real Schur decomposition (16) and hence X from the eigenstructure of H_{symp1} .

This yields an **explicit** numerical method for the reduced RB equations.



The eigenvalues of the matrix H_{symp1} ,

$$H_{\text{symp1}} = \begin{bmatrix} \frac{M}{2} & I \\ \frac{M^2}{4} + J^2 & \frac{M}{2} \end{bmatrix} \quad (17)$$

are the solutions of the **quadratic eigenvalue problem**

$$P(\lambda) = \det(\lambda^2 I - \lambda M - J^2) = 0.$$

Without loss of generality, we assume that J is diagonal, with entries J_1, J_2, J_3 . Then,

$$\begin{aligned} -P(\lambda) &= \lambda^6 - \lambda^4 (J_1^2 + J_2^2 + J_3^2 - m_{12}^2 - m_{13}^2 - m_{23}^2) \\ &\quad + \lambda^2 (J_1^2 J_2^2 + J_1^2 J_3^2 + J_2^2 J_3^2 - m_{12}^2 J_3^2 - m_{13}^2 J_2^2 - m_{23}^2 J_1^2) - J_1^2 J_2^2 J_3^2 \\ &= \lambda^6 - \lambda^4 (\text{tr}(J^2) - \|\mathbf{m}\|_2) + \lambda^2 (C_{J,2} - H_2) - \det(J^2). \end{aligned} \quad (18)$$

$$\begin{aligned} C_{J,i,j} &= J_1^i J_2^j + J_1^i J_3^j + J_2^i J_3^j, \\ C_{J,i} &= C_{J,i,i} \\ C_J &= C_{J,1} \\ H_2 &= (J_1 + J_2)(J_1 + J_3)(J_2 + J_3)H - C_J \|\mathbf{m}\|_2. \end{aligned}$$

- Reduce to a cubic equation (compute the roots explicitly)



Schematical procedure

- Compute eigenvalues/eigenvectors of H_{sympI} :

$$H_{\text{sympI}} \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} = \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} \begin{bmatrix} \Lambda_+ & \\ & \Lambda_- \end{bmatrix}, \quad \text{Re } \Lambda_{\pm} \geq 0,$$

(the eigenvectors need not be orthogonal and may be complex). $Y_1, Y_2 \in \mathbb{R}^{6 \times 3}, \Lambda_{\pm} \in \mathbb{R}^{3 \times 3}$.

- Orthogonalize the eigenvectors (by Gram-Schmidt or QR),

$$[Y_1, Y_2] = QR,$$

so that

$$H_{\text{sympI}}Q = QR\Lambda R^{-1}$$

is the complex Schur form.

- Reduce to a real Schur form by considering real/imaginary part (complex Givens rotation).
- Compute $S = Q_{21}Q_{11}^{-1}, X = (M/2 + S)J^{-1}$.

-
- We don't need all the eigenvectors, just Y_1 . Don't need R .
 - Avoid complex arithmetic altogether.



The numerical DMV algorithm

- $\mathbf{m}_0 \mapsto hM_0 = h\hat{\mathbf{m}}_0$.
- Compute the eigenvalues of $H_{\text{symp1}} = H(M_k)$ solving for $P(\lambda) = 0$ as in (18).
- For $t_k = t_0 + kh$, $k = 0, 1, 2, \dots$
 - Compute the (real) eigenvectors corresponding to Λ_+
 - * Compute 3 'quadratic' eigenvectors (3 matrix factorizations, LU/QR, with pivoting). No need to compute explicitly L or Q .
 - * Compute the 'dependent' eigenvectors.
 - Orthogonalize the eigenspace
 - * By (modified) Gram–Schmidt or QR. Only the Q factor is needed.
 - Compute $S = Q_{21}Q_{11}^{-1}$, $\omega_k = (M/2 + S)J^{-1}$
 - * Update $M_{k+1} = \omega_k^\top M_k \omega_k$
- Rescale $\mathbf{m}_N \leftarrow M_N/h$.

This algorithm produces an explicit method that is about 20 – 22 times more expensive than LP2, the explicit method of McLachlan and Reich.





Concluding remarks

- **Explicit** algorithms to solve for the $N = 3$ free rigid body
- The methods are up to 6th order, completely integrable, possible to increase to arbitrary order
- The cost of the method is about 10 – 22 times more expensive than the explicit LP2. The cheaper versions seem to be less stable especially for large step-size and long time computations
- Reconstruction equations: Find the configuration

$$X_{k+1} = X_k \omega_k^\top.$$

The complexive order is still 2 but the error is generally smaller. Backward error analysis reveals that some error terms cancel, however the components are reparametrized with 3 different time scales.

To obtain higher order reconstructions, one can use interpolation of the vector field $X\Omega$ and its higher derivatives using the computed values of Ω_k .

- Optimal step-size?





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