An explicit, completely integrable, second-order method for the 3x3 rigid body

This talk is based on a work done in CAS, Oslo, in collaboration with Robert McLachlan.

Antonella Zanna
University of Bergen, Norway

email: anto@ii.uib.no
http://www.ii.uib.no/˜anto

Overview

- The Moser–Veselov discrete rigid body
- On the solution of the matrix equation $M = \omega^\top J - J\omega$
- Explicit methods for the 3×3 case
- Numerical experiments and comparisons with other methods

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

Consider the fuctional $S(X)$ determined by

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

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

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

(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 left and taking into consideration the symmetry of Λ_k,

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

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 $\omega_k = X_k^\top X_{k-1} \in \mathrm{O}(N)$ 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), (1) becomes

$$\begin{aligned} M_{k+1} &= \omega_k M_k \omega_k^\top \\ M_k &= \omega_k^\top J - J\omega_k. \end{aligned} \tag{2}$$

the **discrete Euler–Arnold** equation.

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

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

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

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

To solve the discrete Euler–Arnold equations (2):

- For $k = 0, 1, 2, \ldots$, find $\omega_k \in \mathfrak{so}(N)$ 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

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

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

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

Note that

- Marsden, Pekarsky & Skoller (1999) also arrive to an analogous discrete map via a discrete Lie–Poisson (DEP) algorithm.
- Also the IMR is second order, preserves the Poisson structure and all the integrals of the continuous rigid body.

Solving the Moser–Veselov equation

The core of this talk is how to solve numerically the Moser–Veselov equation

$$M = \omega^\top J - J\omega, \qquad M^\top = -M, \quad \omega^\top \omega = I. \tag{3}$$

- The Moser–Veselov equation (3) has not a unique solution;
- However, if the set S of eigenvalues ν of $W = \omega^\top J$ admits a splitting $S = S_+ \cup S_-$, with

  $$\bar{S}_+ = S_+, \qquad \bar{S}_- = S_-, \qquad S_- = -S_+, \qquad S_+ \cap S_- = \emptyset, \tag{4}$$

  then, there exists a unique $\omega = JW^{-1}$ that satisfies (3), with $\mathrm{spec} W = S_+$ (Moser & Veselov 1991).

We recall that the eigenvalues ν are the solutions of the characteristic equation

$$P(\nu) = \det(\nu^2 I - \nu M - J^2) = 0. \tag{5}$$

Connections with matrix Riccati equations

Consider the matrix equation

$$M = XJ - JX^{\top}. \tag{6}$$

Cardoso & Leite (2001) shown that every solution of (6) (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 (6) if and only if S is a symmetric solution of the Riccati equation

$$S^2 + S(M/2) + (M/2)^{\top}S - (M^2/4 + J^2) = 0. \tag{7}$$

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

$$H = \begin{bmatrix} \frac{M}{2} & I \\ \frac{M^2}{4} + J^2 & \frac{M}{2} \end{bmatrix}. \tag{8}$$

If $\frac{M^2}{4} + J^2$ is positive definite, it has been shown in (Cardoso & Leite 2001) that (7) 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

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

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Algorithm(Cardoso & Leite 2001): Compute X, the unique solution of (6) in the special orthogonal group $\mathrm{SO}(n)$.

1. Find a real Schur form of H,

$$\tilde{Q}^\top H \tilde{Q} = \begin{bmatrix} T_{11} & T_{12} \\ O & T_{22} \end{bmatrix}, \tag{9}$$

   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.

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The case $N = 3$

In this case,

- it is possible to find an **explicit spectral decomposition** of H (without the QR eigenvalue method)
- construct the real Schur decomposition (9) and hence X from the eigenstructure of H.

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

The eigenvalues of the matrix H,

$$H = \begin{bmatrix} \frac{M}{2} & I \\ \frac{M^2}{4} + J^2 & \frac{M}{2} \end{bmatrix} \tag{10}$$

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,

$$\begin{aligned} -P(\lambda) = \lambda^6 - \lambda^4 \left(J_1^2 + J_2^2 + J_3^2 - m_{12}^2 - m_{13}^2 - m_{23}^2\right) \\ + \lambda^2 \left(J_1^2 J_2^2 + J_1^2 J_3^2 + J_2^2 J_3^2 - m_{12}^2 J_3^2 - m_{13}^2 J_2^2 - m_{23}^2 J_1^2\right) - J_1^2 J_2^2 J_3^2. \end{aligned} \tag{11}$$

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

Schematical procedure

- Compute eigenvalues/eigenvectors of H:

$$H \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} = \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} \begin{bmatrix} \Lambda_+ & \\ & \Lambda_- \end{bmatrix}, \qquad \operatorname{Re}\Lambda_+ \geq 0,$$

  (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 Grahm-Schmidt or QR),

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

  so that

$$HQ = QR\Lambda R^{-1}$$

  is the complex Schur form.

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

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

Practical computation of the spectral decomposition Assume that $H\mathbf{y} = \lambda\mathbf{y}$, where $\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathrm{quad}} \\ \mathbf{y}_{\mathrm{d}} \end{bmatrix}$ and H is as in (10). Then,

$$(J^2 - \lambda M - \lambda^2 I)\mathbf{y}_{\mathrm{quad}} = \mathbf{0},$$

while

$$\frac{M}{2}\mathbf{y}_{\mathrm{quad}} + \mathbf{y}_{\mathrm{d}} = \lambda I.$$

Complex eigenvalues: If $\lambda = \mu + \mathrm{i}\nu$ and

$$\mathbf{y} = \mathbf{u} + \mathrm{i}\mathbf{v}$$

then, separating real and imaginary part,

$$\begin{bmatrix} J^2 + \mu M + (\nu^2 - \mu^2)I & -\nu M + 2\mu\nu I \\ \nu M - 2\mu\nu I & J^2 + \mu M + (\nu^2 - \mu^2)I \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathrm{quad}} \\ \mathbf{v}_{\mathrm{quad}} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix},$$

for the eigenvectors of the quadratic eigenvalue problem.
Similarly, for the 'dependent' components,

$$\begin{aligned} \frac{M}{2}\mathbf{u}_{\mathrm{quad}} + \mathbf{u}_{\mathrm{d}} &= \mu\mathbf{u}_{\mathrm{quad}} - \nu\mathbf{v}_{\mathrm{quad}} \\ \frac{M}{2}\mathbf{v}_{\mathrm{quad}} + \mathbf{v}_{\mathrm{d}} &= \nu\mathbf{u}_{\mathrm{quad}} + \mu\mathbf{v}_{\mathrm{quad}}. \end{aligned}$$

The numerical algorithm

For $t_k = t_0 + kh$, $k = 0, 1, 2 \ldots$

- Compute the eigenvalues of $H = H(M_k)$
  - $P(\lambda)$ as in (11). Only $m_{ij}^2 J_k^2$ needs be recomputed
- Compute the (real) eigenvectors corresponding to Λ_+
  - Compute 3 'quadratic' eigenvectors (3 matrix factorizations, LU/QR, with pivoting). No need to compute explicitely L or Q.
  - Compute the 'dependent' eigenvectors.
- Orthogonalize the eigenspace
  - By (modified) Grahm–Schmidt or QR. Only the Q factor is needed.
- Compute $\quad S = Q_{21} Q_{11}^{-1}, \quad \omega_k = (M/2 + S) J^{-1}$
  - In the 3×3 case, explicit computation of the inverse is computationally cheaper.
- Update $M_{k+1} = \omega_k^\top M_k \omega_k$

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 Moser–Veselov explicit scheme with the Hamiltonian-splitting method of (McLachlan 1993)

$$H = \frac{m_1^2}{J_{2,2} + J_{3,3}} + \frac{m_2^2}{J_{1,1} + J_{3,3}} + \frac{m_3^2}{J_{1,1} + J_{2,2}} = H_1 + H_2 + H_3$$

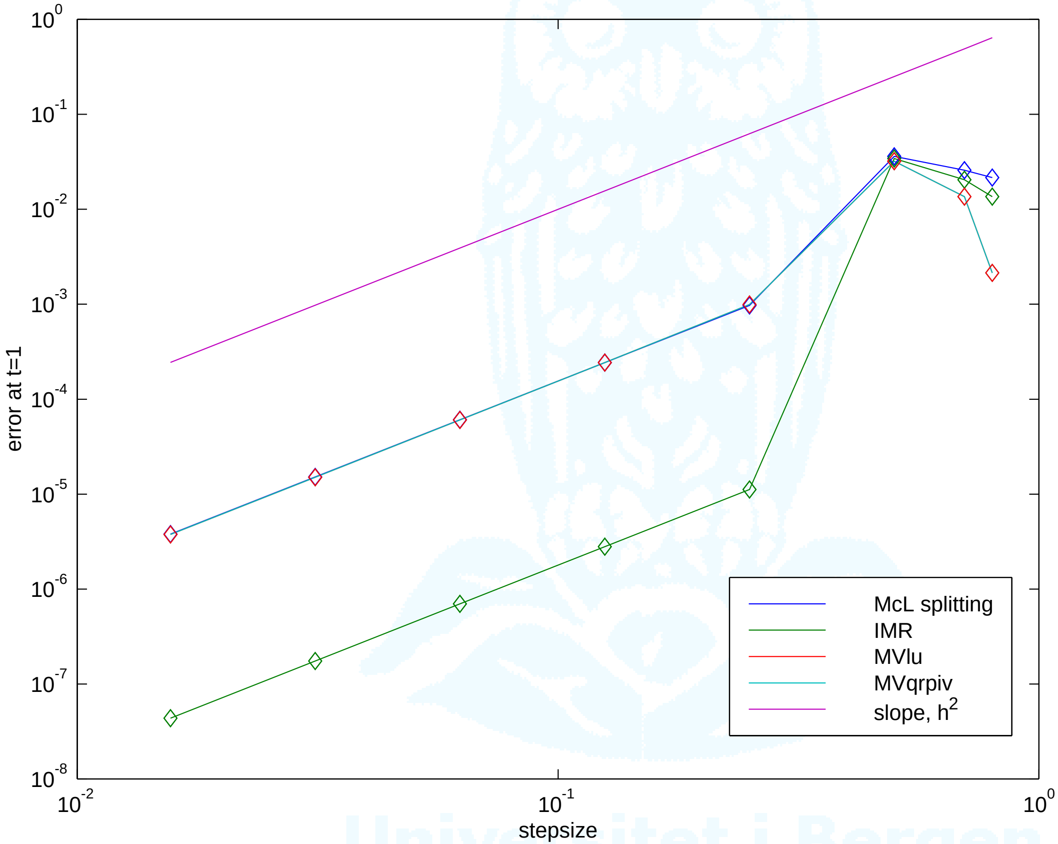
and the Implicit Midpoint Rule (IMR),

$$\mathbf{m}_{k+1} = \mathbf{m}_k + h\mathbf{f}(\frac{\mathbf{m}_k + \mathbf{m}_{k+1}}{2}),$$

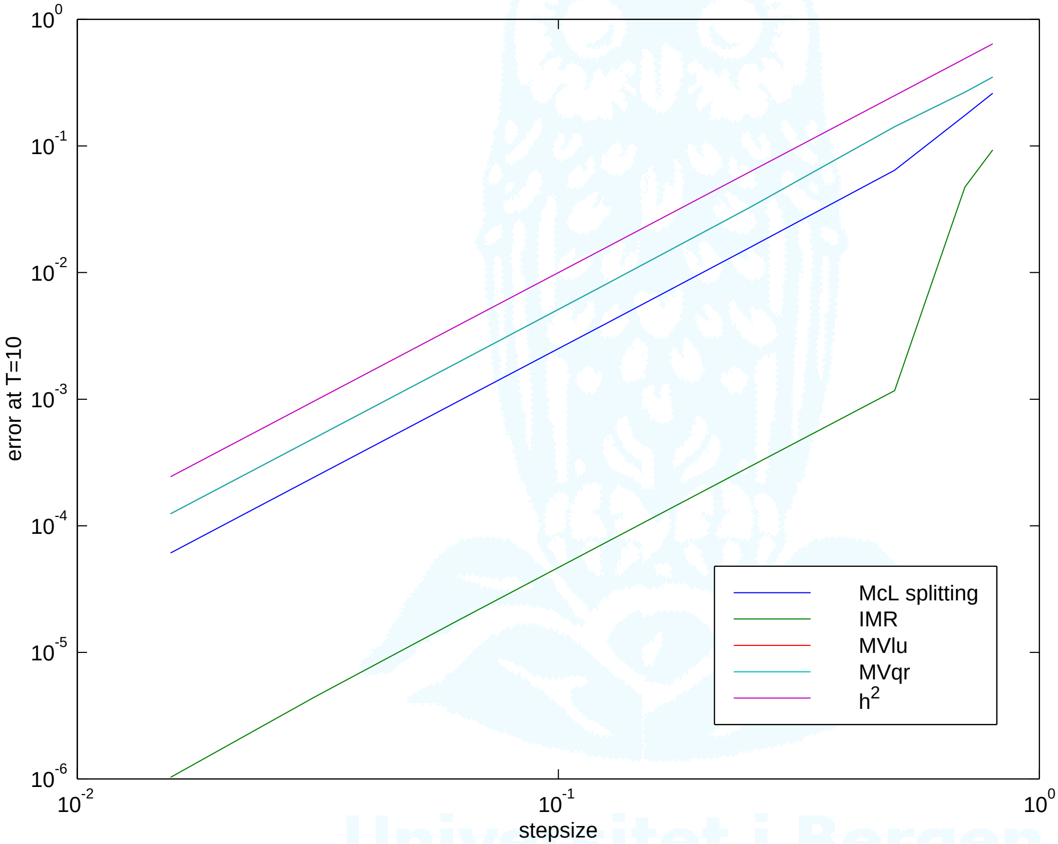
where

$$\mathbf{f}(\mathbf{m}) = \mathbf{m} \times (\tilde{J})^{-1}\mathbf{m}, \qquad \tilde{J} = \begin{bmatrix} J_{2,2} + J_{3,3} & 0 & 0 \\ 0 & J_{1,1} + J_{3,3} & 0 \\ 0 & 0 & J_{1,1} + J_{2,2} \end{bmatrix}.$$

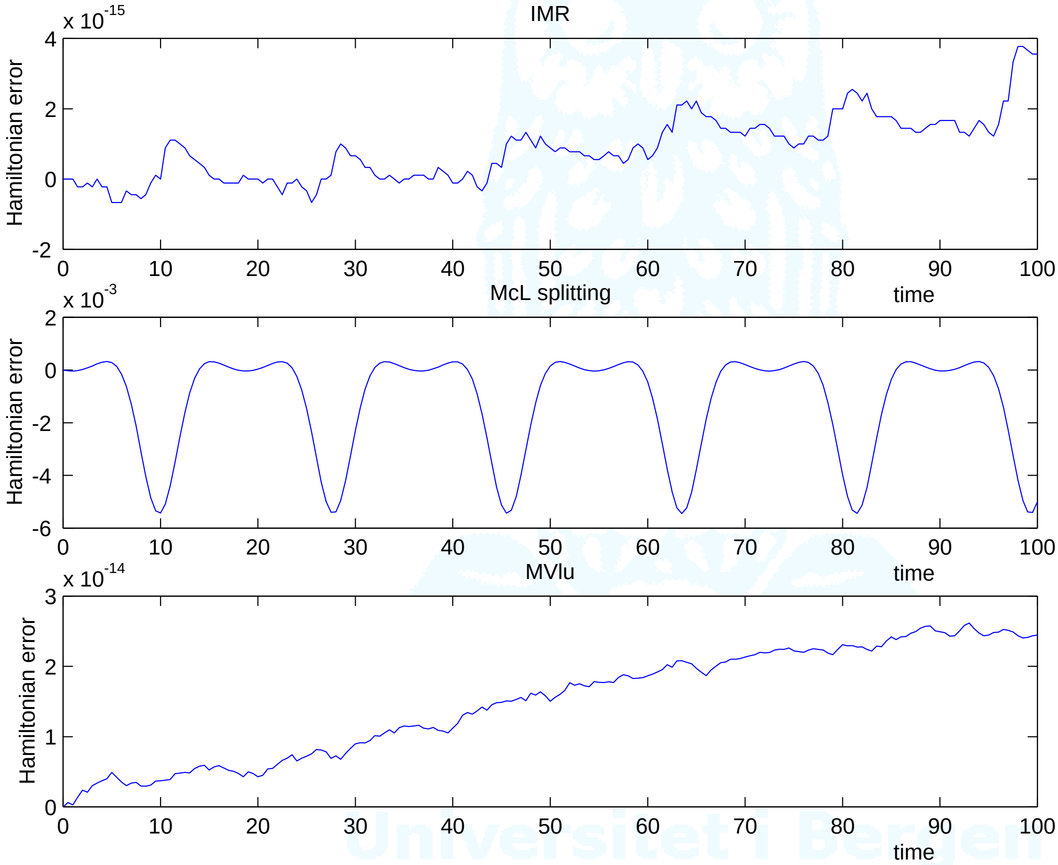
Error of the methods at $t = 1$ for various stepsizes



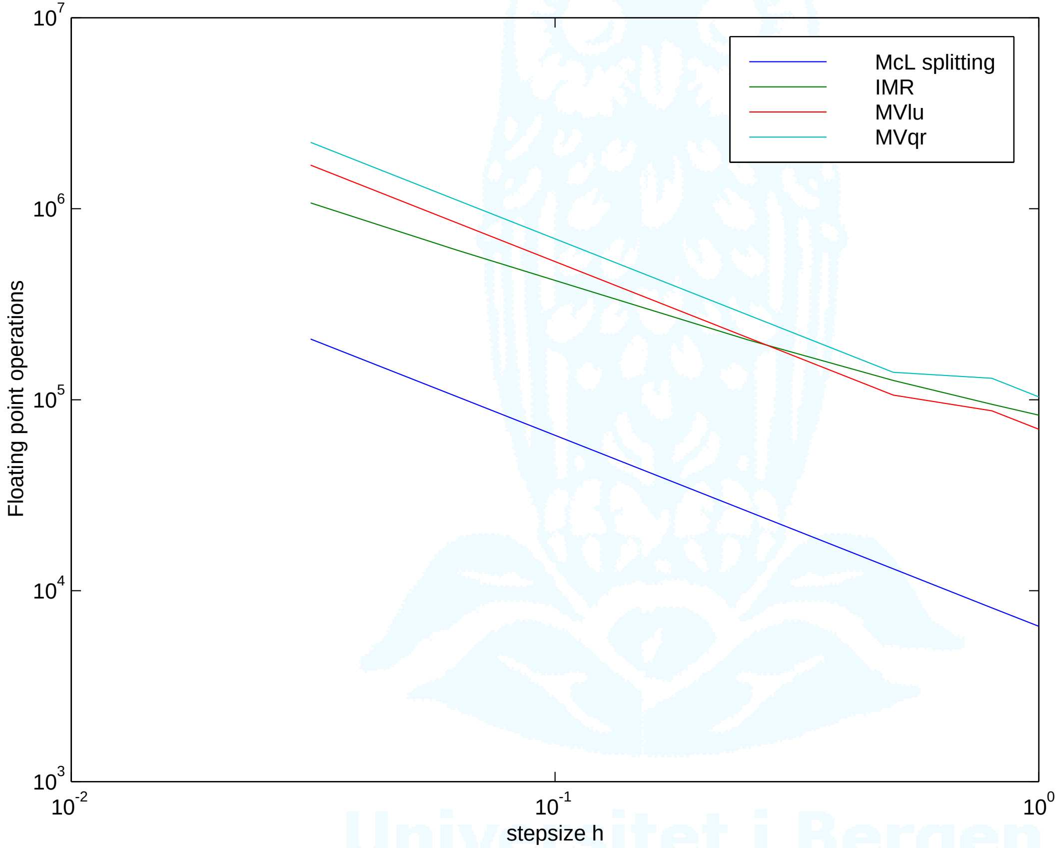
Error of the methods at $t = 10$ for various stepsizes



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



Floating point operations versus stepsize in the interval $[0, 100]$.



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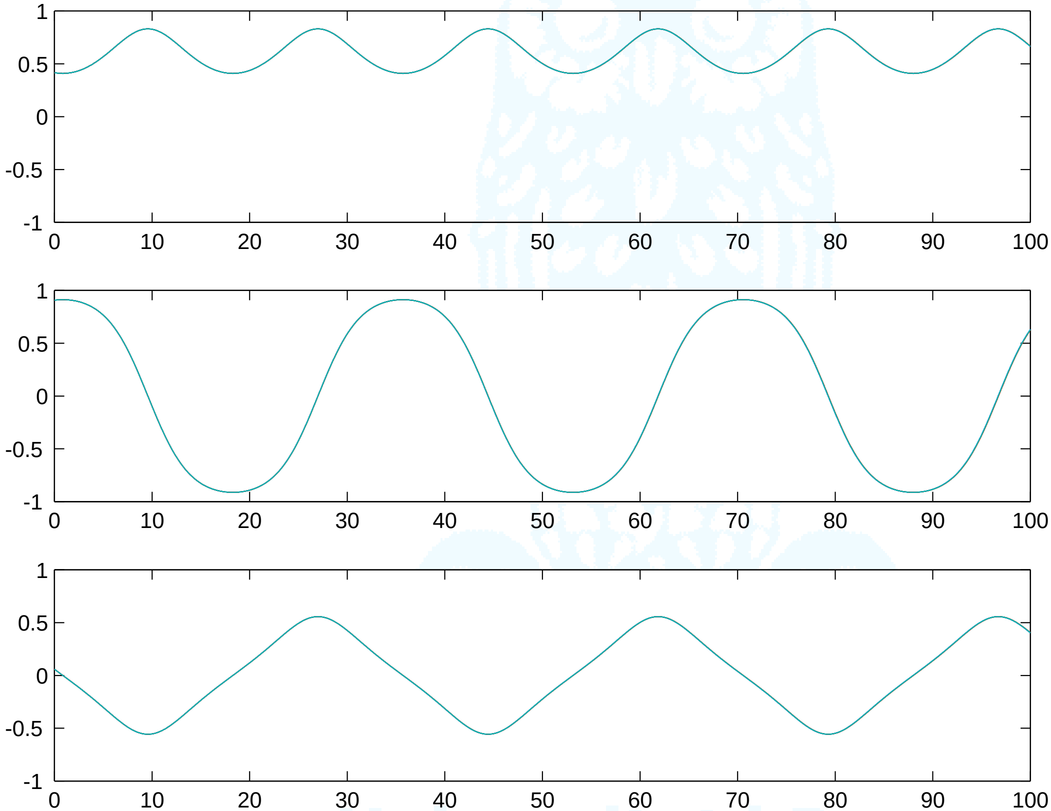
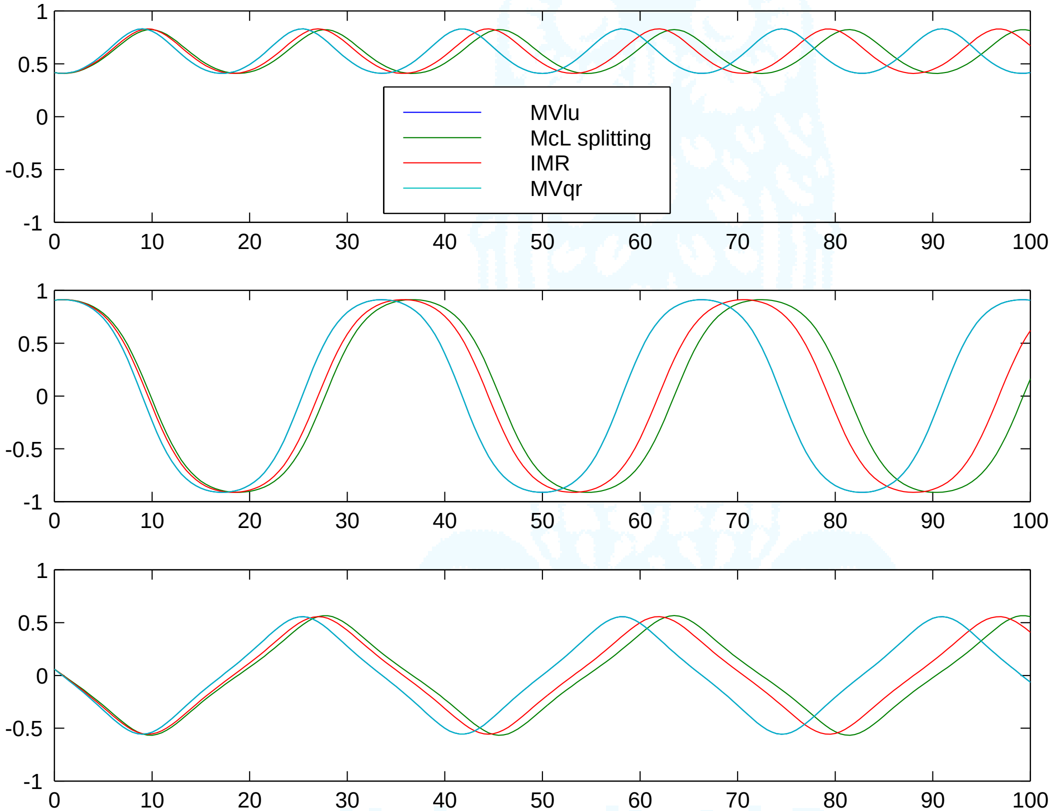
The components of the vector $\mathbf{m}_k$ for $h = \frac{1}{10}\ldots$



. . . and for $h = \frac{1}{2}$ . . .



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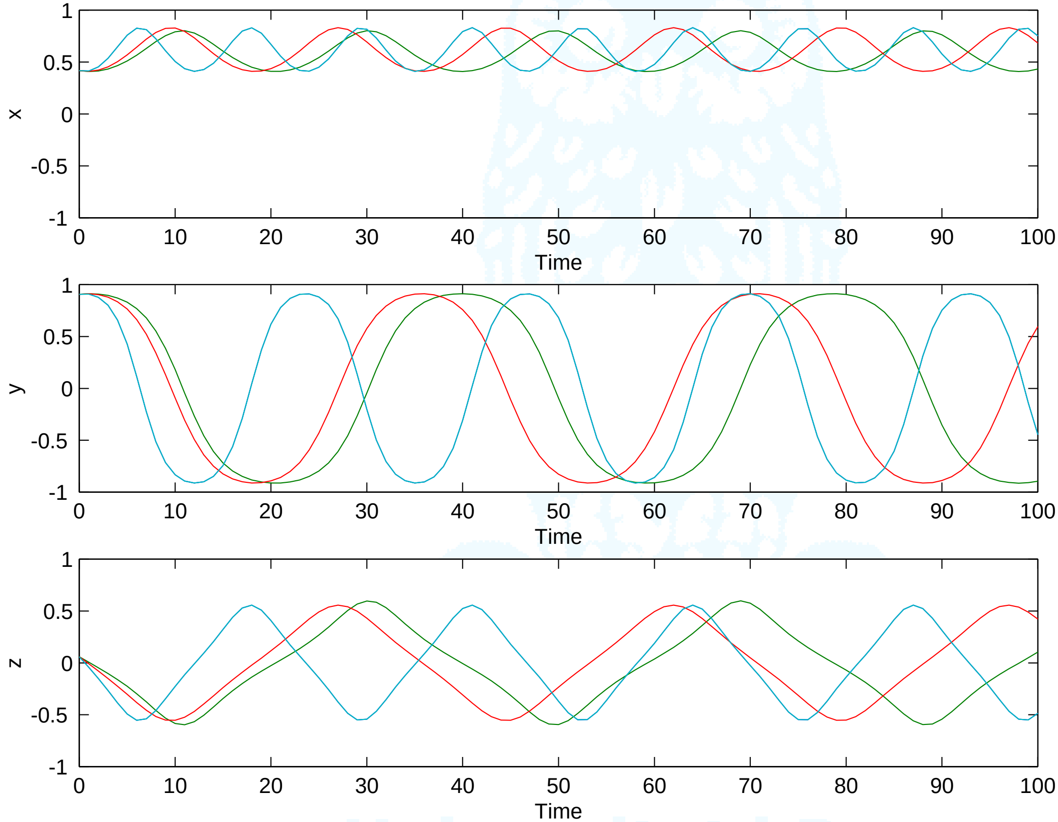
. . . and for $h = 1$ . . .



Concluding remarks

- A new **explicit** method for the $N = 3$ rigid body
- The method is 2nd order, completely integrable
- Comparable in cost with the IMR but ≈ 10 more expensive than the McL-splitting
- For larger step-size (when it is cheaper than IMR) it appears to have larger errors
- Open problems:
  - Is it possible to make this even cheaper?
  - More extensive testing, with different initial conditions and inertia tensors is needed

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