Colloque Numérique Suisse Fribourg, April 2008

High-order numerical integrators based on modified differential equations

Gilles Vilmart

(INRIA Rennes & Univ. Genève)

PhD under the directorship of

Philippe Chartier and Ernst Hairer

Plan of the talk

- Main ideas of the **theory of modified differential equations** for the study of geometric integrators.

- We derive efficient high-order **rigid body integrators**.

  Preprocessed Discrete Moser–Veselov algorithm.

- Reducing **round-off errors** in long time integration.

  algorithm based on Jacobi elliptic functions.

Geometric Numerical Integration

A two-dimensional Hamiltonian system,

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\nabla V(q) \end{aligned}$$

with a quartic potential $V(q) = (q^2 - 1)^2$.

$$\text{Hamiltonian } H(q,p) = \tfrac{1}{2}p^2 + (q^2 - 1)^2.$$

$\longrightarrow$ animation

Studied recently in the context of the computation of conjugate points for the Martinet case in optimal control.

M. Chyba, E. Hairer, G. Vilmart, **The role of symplectic integrators in optimal control**, to appear in Optimal control, applications and methods, 2008

Free rigid body equations

$$\dot{y} = \widehat{y}\, I^{-1} y, \quad \dot{Q} = Q\, \widehat{I^{-1} y}, \qquad \widehat{a} = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}$$

where $I = \mathsf{diag}(I_1, I_2, I_3)$ are the moments of inertia.

$y = (y_1, y_2, y_3)^T$ angular momentum, Q orthogonal matrix.

Free rigid body equations

$$\dot{y} = \widehat{y}\, I^{-1} y, \qquad \dot{Q} = Q\, \widehat{I^{-1} y}, \qquad\qquad \widehat{a} = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}$$

where $I = \mathsf{diag}(I_1, I_2, I_3)$ are the moments of inertia.

$y = (y_1, y_2, y_3)^T$ angular momentum, Q orthogonal matrix.

First integrals: $\quad Qy$,

$$H(y) = \frac{1}{2}\Big(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\Big) \quad \text{and} \quad C(y) = \frac{1}{2}\Big(y_1^2 + y_2^2 + y_3^2\Big).$$

(Hamiltonian and Casimir)

Discrete Moser–Veselov algorithm

$$\dot y = \widehat{y}\, I^{-1} y, \qquad \dot Q = Q\, \widehat{I^{-1} y}, \qquad\qquad \widehat{a} = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}$$

DMV (1991) We consider $D = \mathsf{diag}(d_1, d_2, d_3)$ where

$$d_1 + d_2 = I_3, \qquad d_2 + d_3 = I_1, \qquad d_3 + d_1 = I_2,$$

For given (y_n, Q_n), compute an orthogonal matrix ω_n from

$$\omega_n^T D - D\omega_n = h\, \widehat{y}_n$$

The numerical solution after one step is then given by

$$\widehat{y}_{n+1} = \omega_n\, \widehat{y}_n\, \omega_n^T, \qquad\qquad Q_{n+1} = Q_n\, \omega_n^T.$$

It is symmetric, symplectic, Poisson, and it exactly preserves all first integrals. The only drawback is its low order 2.

Preprocessed DMV algorithm

Apply the DMV algorithm (order 2) with I_j replaced by $\widetilde{I}_j$ where

$$\frac{1}{\widetilde{I}_j} = \frac{1}{I_j}\Big(1 + h^2 s_3(y_n) + \ldots + h^{2r-2} s_{2r-1}(y_n)\Big) \\ + h^2 d_3(y_n) + \ldots + h^{2r-2} d_{2r-1}(y_n)$$

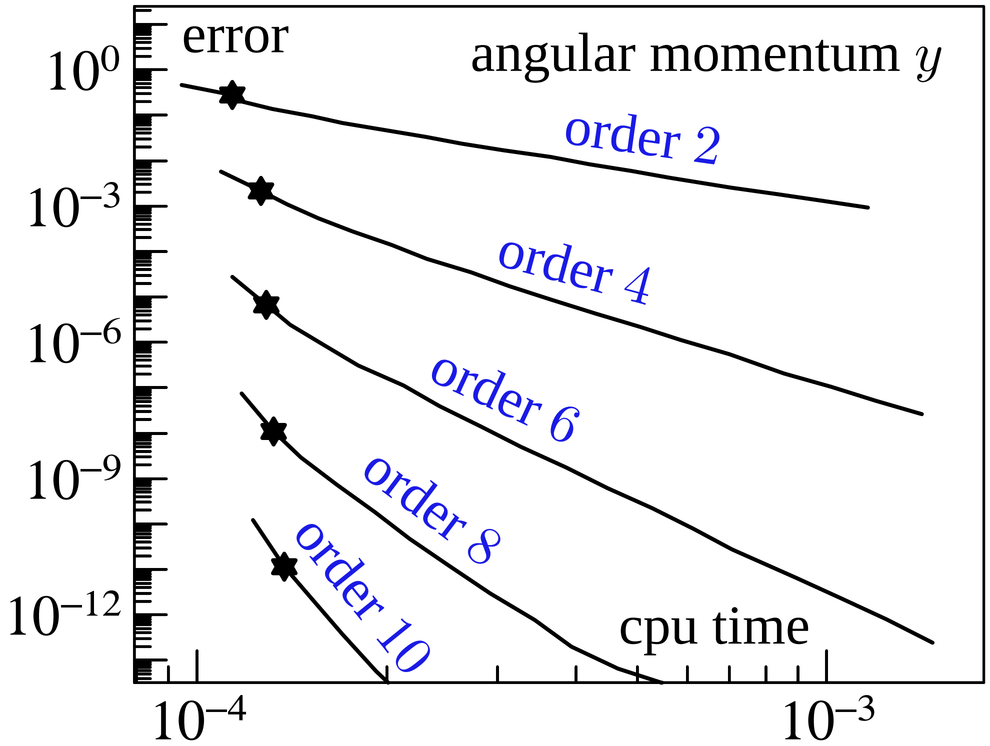
to get an integrator of order $2r$.

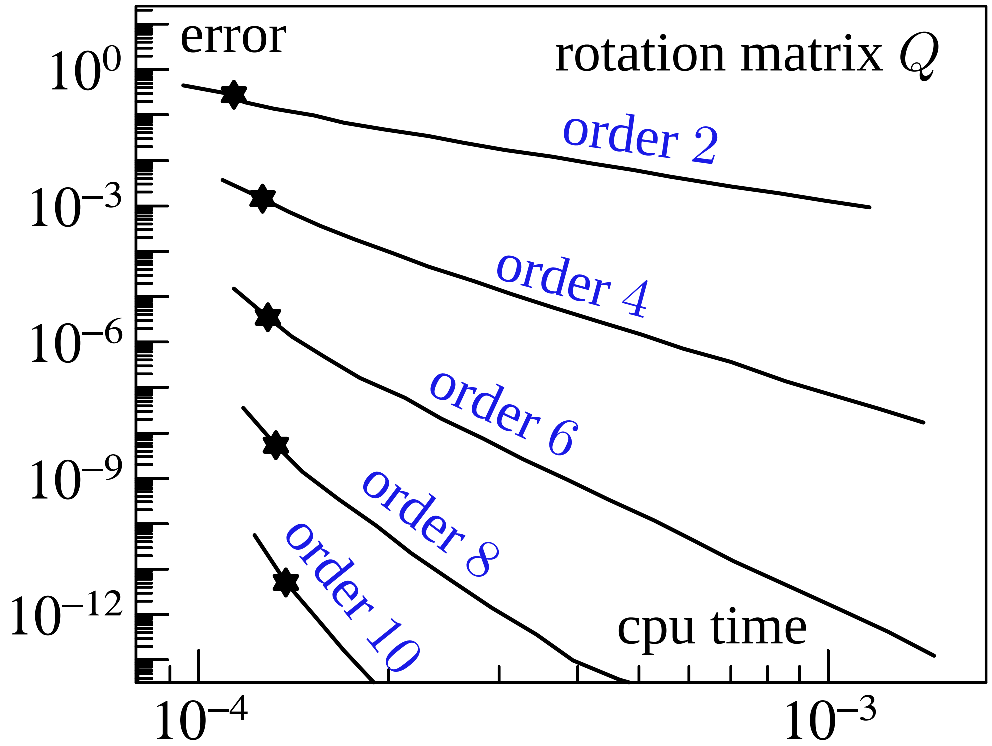
$$\begin{aligned} s_3(y_n) &= -\frac{1}{3}\Big(\frac{1}{I_1} + \frac{1}{I_2} + \frac{1}{I_3}\Big) H(y_n) + \frac{I_1 + I_2 + I_3}{6\, I_1\, I_2\, I_3} C(y_n), \\ d_3(y_n) &= \frac{I_1 + I_2 + I_3}{6\, I_1\, I_2\, I_3} H(y_n) - \frac{1}{3\, I_1\, I_2\, I_3} C(y_n). \end{aligned}$$

E. Hairer, G. Vilmart, **Preprocessed Discrete Moser-Veselov algorithm for the full dynamics of the free rigid body**, J. Phys. A, 2006.

Numerical experiment

asymmetric rigid body: $I_1 = 0.6, \; I_2 = 0.8, \; I_3 = 1.0$

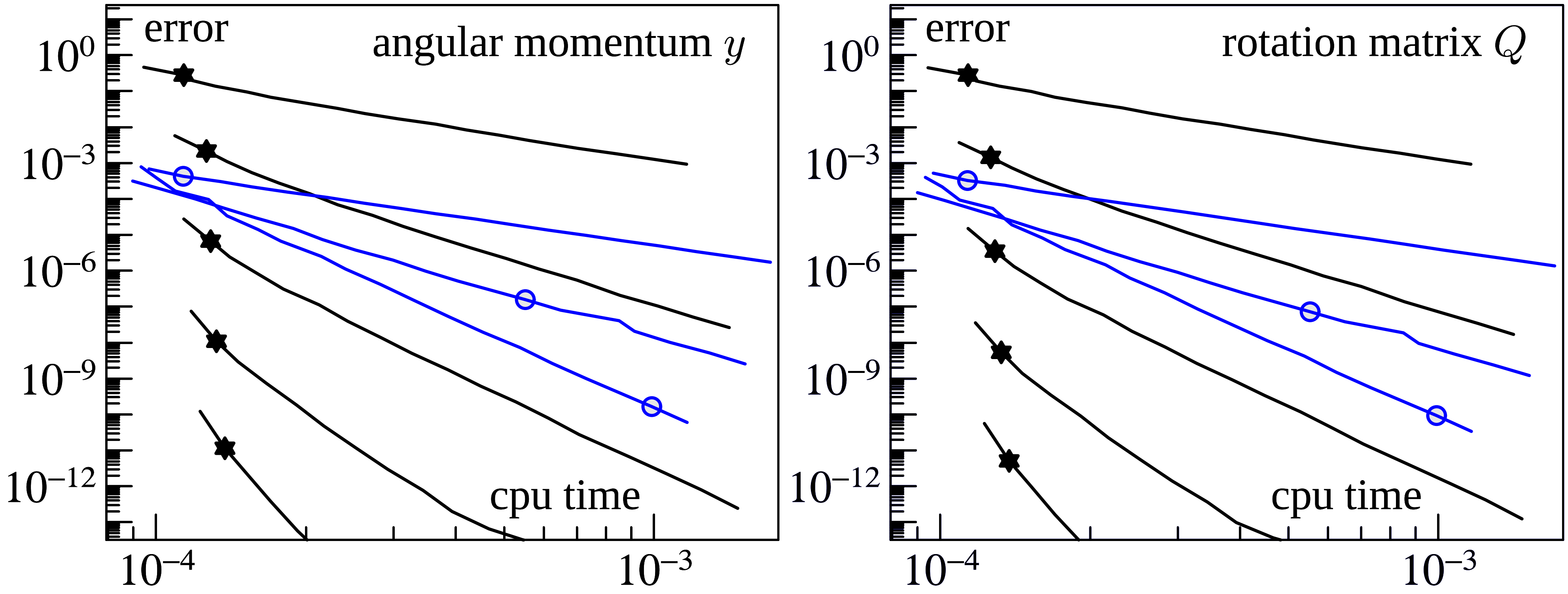




preprocessed DMV of orders 2, 4, 6, 8, 10

Numerical experiment

asymmetric rigid body: $I_1 = 0.6,\ I_2 = 0.8,\ I_3 = 1.0$



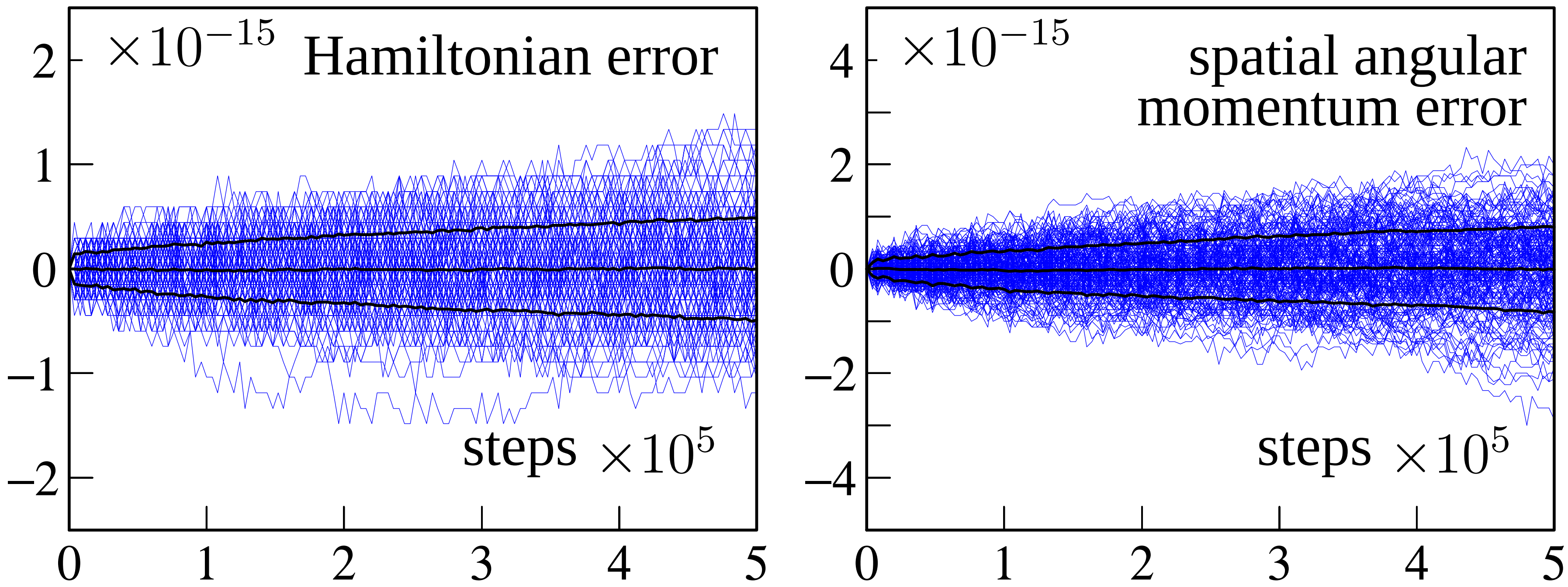
blue: splitting methods of orders 2, 4, 6 (composition methods)

black: preprocessed DMV of orders 2, 4, 6, 8, 10

Study of roundoff errors propagation: the DMV algorithm

Probabilistic model (Henrici, 1962): in the absence of a deterministic source of errors, roundoff errors behave like a random walk:

$$\text{Hamiltonian error } = \mathcal{O}(eps\sqrt{h}\sqrt{t})$$

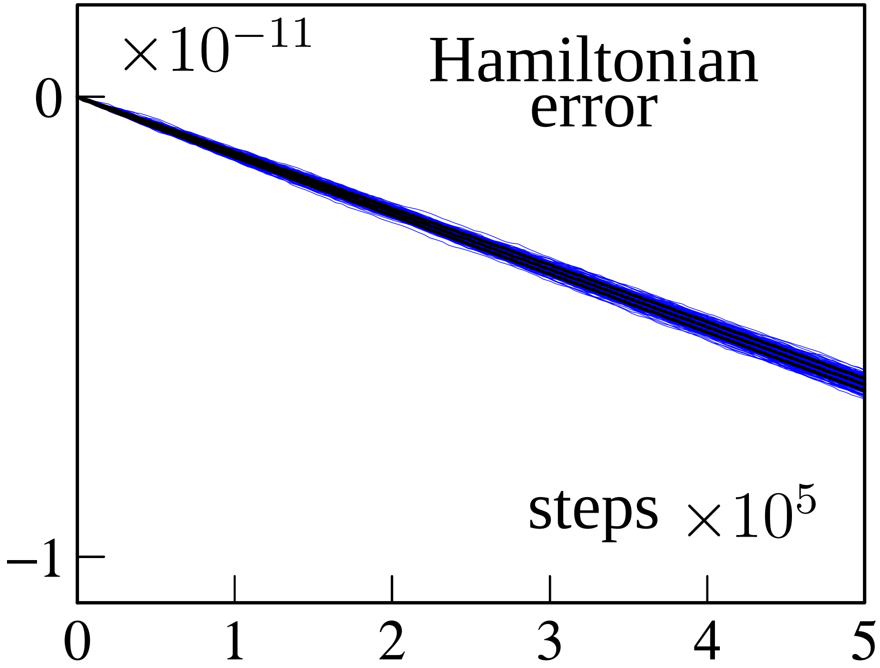


Integrators based Jacobi elliptic functions

In several recent publications (2006, 2007), it is proposed to integrate the rigid body motion using Jacobi elliptic functions. This approach analytically yields the exact solution. However, a standard implementation shows an unexpected propagation of round-off errors.

Integrators based Jacobi elliptic functions

In several recent publications (2006, 2007), it is proposed to integrate the rigid body motion using Jacobi elliptic functions. This approach analytically yields the exact solution. However, a standard implementation shows an unexpected propagation of round-off errors.



Error per step: $\approx 1.25 \times 10^{-17}$

(machine precision $eps = 2^{-53} \approx 2 \times 10^{-16}$)

Explanation: inexact coefficients

The integrator based on Jacobi elliptic functions uses many constants depending en I_1, I_2, I_3, e.g.

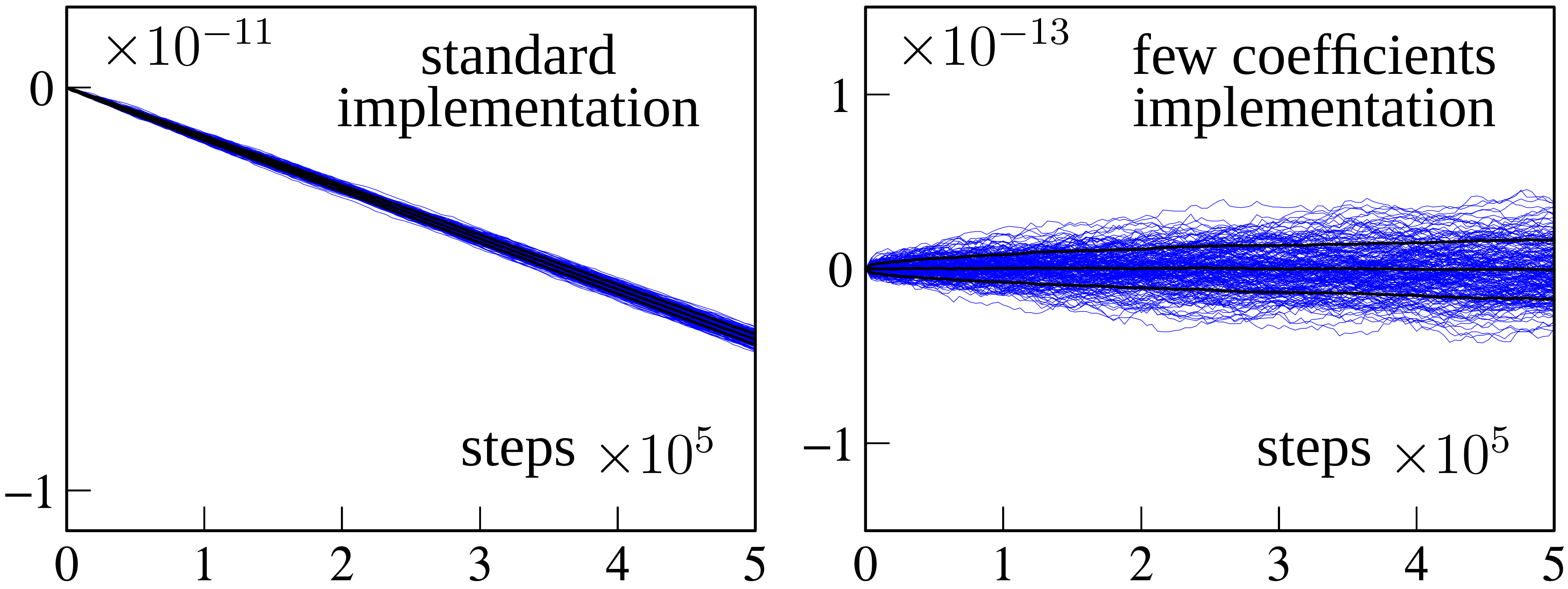
$$
\begin{aligned}
y_1(t) &= c_1 a_1 \mathrm{cn}(u,k), \quad y_2(t) = c_2 a_1 \mathrm{sn}(u,k), \quad y_3(t) = \delta c_3 a_2 \mathrm{dn}(u,k), \\
c_1 &= \sqrt{I_1/(I_3 - I_1)}, \quad c_2 = \ldots, \quad c_3 = \ldots \\
a_1 &= \sqrt{2H(y) I_3 - 2C(y)}, \quad a_2 = \ldots, \\
u &= \sqrt{(I_3 - I_2)/(I_1 I_2 I_3)}\,\delta a_2 t + \ldots \quad k = \ldots
\end{aligned}
$$

The same rounded coefficients are used along the integration.

In (E. Hairer, R. I. McLachlan & A. Razakarivony, 2007), it is shown that for implicit Runge-Kutta methods, if rounded coefficients a_{ij} and b_j are used, then the order conditions are not exactly satisfied, and this induces a systematic error in long-time integrations.

New implementation

To reduce the effect of rounding errors, the main idea is to rewrite the algorithm so that only 3 constants depending on I_1, I_2, I_3 are involved.



G. Vilmart, **Reducing round-off errors in rigid body dynamics**, to appear in Journal of Computational Physics, 2008.