Journées Michel Crouzeix, juin 2006

Modified differential equations

Ernst Hairer, Geneva

This is joint work with

Philippe Chartier and Gilles Vilmart

based on the monograph GNI written with

Christian Lubich and Gerhard Wanner

Program of the talk

Extending and combining the ideas of two well-established theories

- backward error analysis (modified equations),
- Hamilton–Jacobi theory (generating functions),

we derive new, efficient integrators

- preprocessed vector field integrators

for rigid body simulations.

1. Backward error analysis

Given a differential equation

$$\dot{y} = f(y), \quad y(0) = y_0$$

and a numerical one-step method

$$y_{n+1} = \Phi_h(y_n).$$

Find a modified differential equation

$$\dot{z} = f(z) + hf_2(z) + h^2 f_3(z) + h^3 f_4(z) + \ldots$$

such that for $t_n = nh$,

$$\boxed{y_n = z(t_n)}$$

Origin and references

Numerical linear algebra

Wilkinson 1960, Turing award 1970

Numerical ordinary differential equations

formal considerations

Ruth 1983, Gladman, Duncan & Candy 1991,

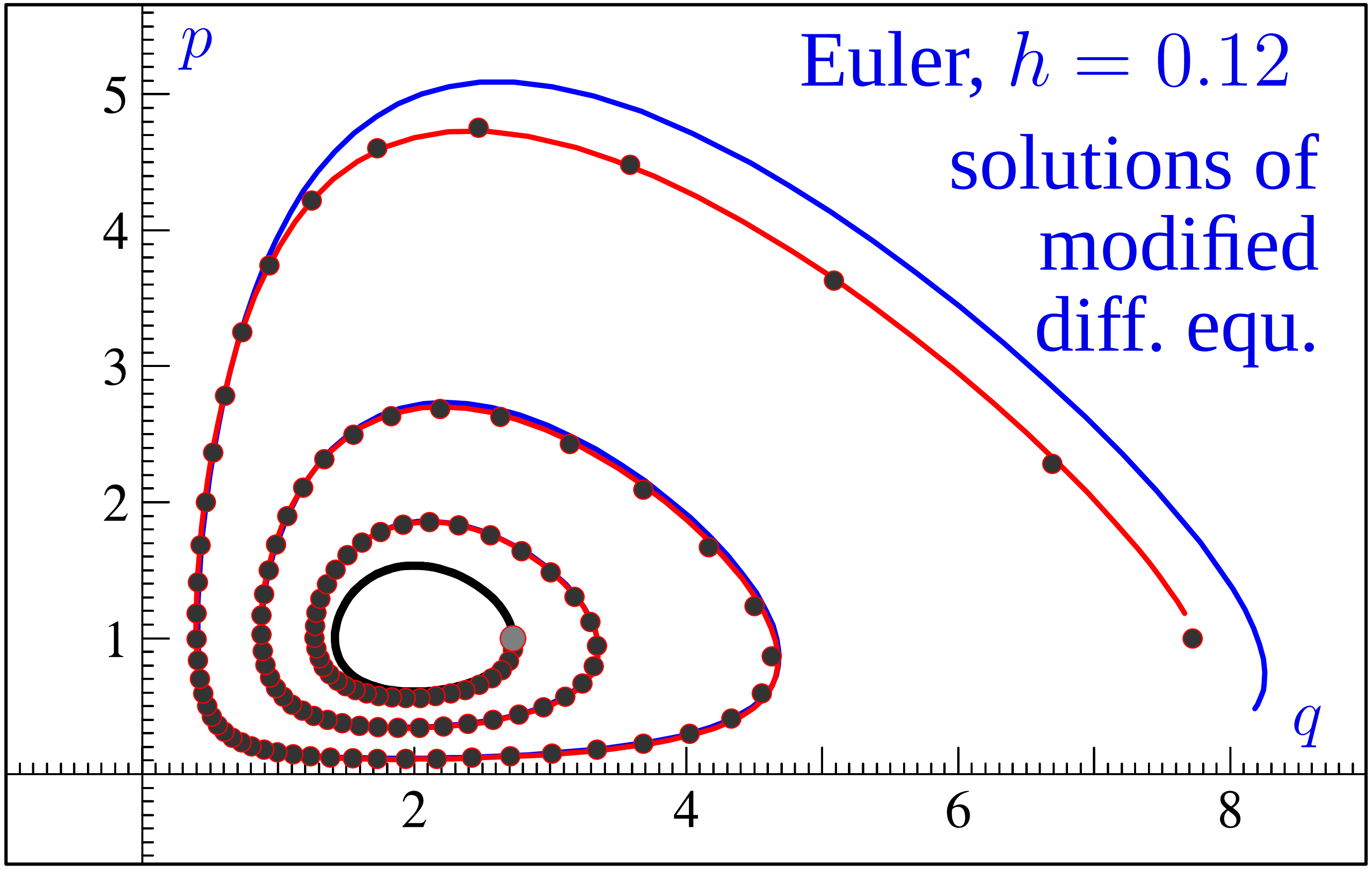
systematic study

Griffiths & Sanz-Serna 1986, Feng 1991,
Sanz-Serna 1991, Yoshida 1993, Eirola 1993,
Fiedler & Scheurle 1996

rigorous analysis

Benettin & Giorgilli 1994, H. & Lubich 1997,
Reich 1999

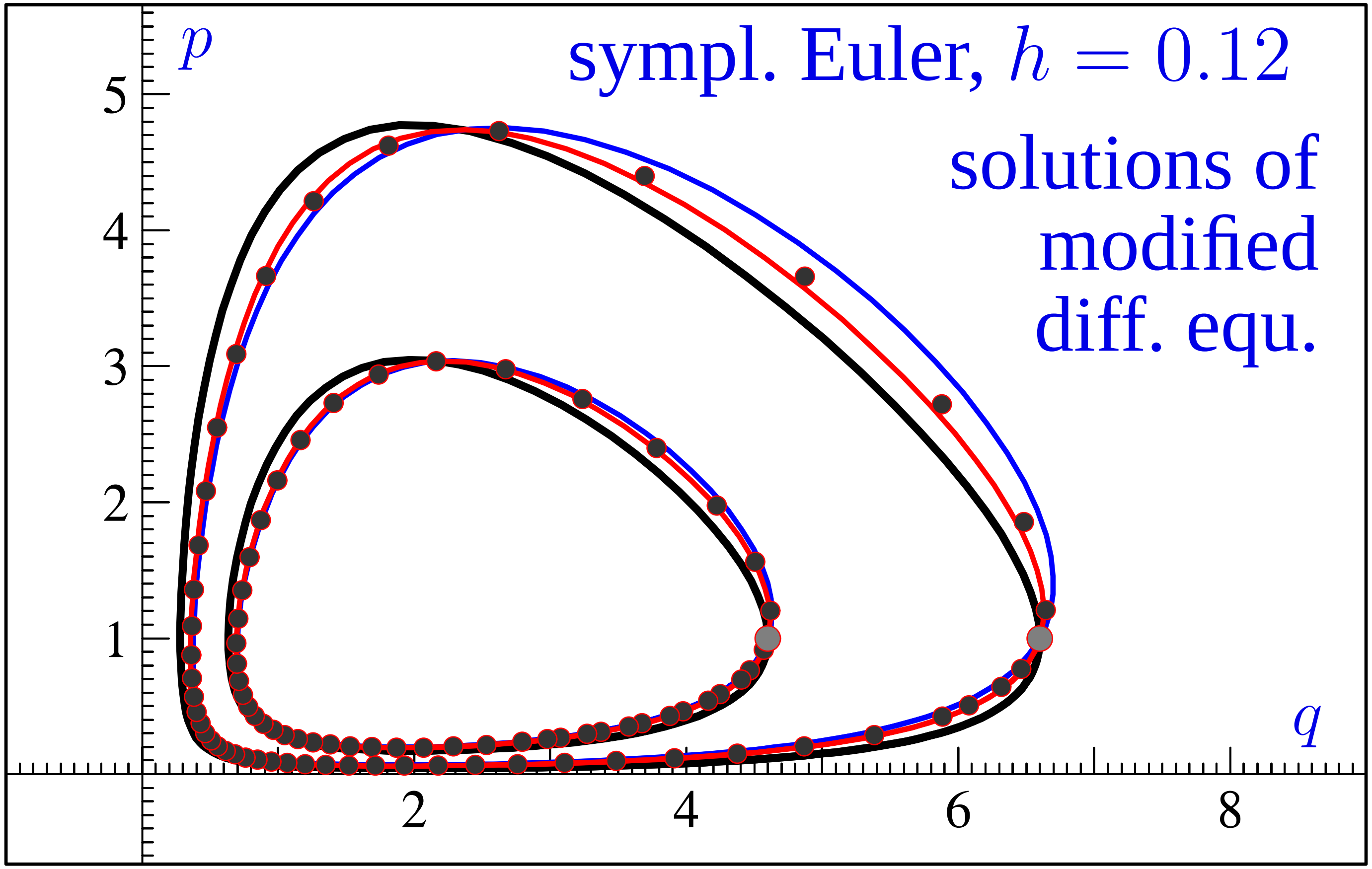
Example 1: Lotka–Volterra and explicit Euler



$$\dot{q} = q(p-1), \qquad q_{n+1} = q_n + h\, q_n(p_n - 1)$$

$$\dot{p} = p(2-q), \qquad p_{n+1} = p_n + h\, p_n(2 - q_n)$$

Example 2: Lotka–Volterra and symplectic Euler



$$\dot{q} = q(p-1), \qquad q_{n+1} = q_n + h\, q_n(p_{n+1} - 1)$$

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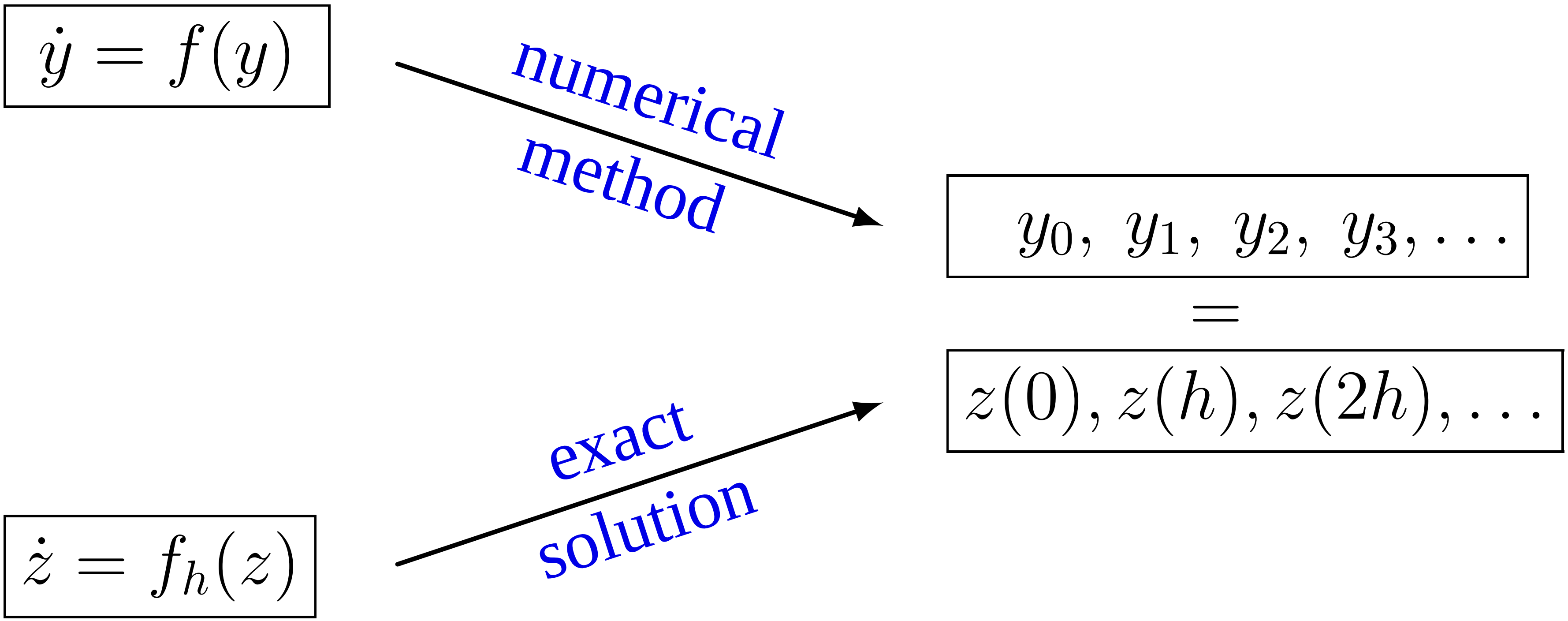
Summary of backward error analysis



modified differential equation

$$\dot{z} = f_h(z) = f(z) + h f_2(z) + h^2 f_3(z) + \ldots$$

2. Hamilton–Jacobi theory

"... Professor Hamilton hat ... das merkwürdige Resultat gefunden, dass ... sich die Integralgleichungen der Bewegung ... sämmtlich durch die partiellen Differentialquotienten einer einzigen Function darstellen lassen. (C.G.J. Jacobi, 1837)

For a Hamiltonian system

$$\dot{p} = -\nabla_q H(p, q), \qquad \dot{q} = \nabla_p H(p, q)$$

the flow $(p, q) \mapsto (P, Q)$ is symplectic: $P\,dQ - p\,dq \;=\; dS$,
and can be expressed as

$$P = \nabla_Q S(q, Q, t), \qquad p = -\nabla_q S(q, Q, t)$$

where (Hamilton–Jacobi differential equation)

$$\frac{\partial S(q, Q, t)}{\partial t} + H\Big(\nabla_Q S(q, Q, t), Q\Big) = 0$$

We reformulate these formulas:

a) we consider (P, q) as independent variables;

b) we let $S^1(P, q, t) = P(Q - q) - S(q, Q, t)$

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The exact flow $(p, q) \mapsto (P, Q)$ of the Hamiltonian system

$$\dot{p} = -\nabla_q H(p, q), \qquad \dot{q} = \nabla_p H(p, q)$$

is given by

$$P = p - \nabla_q S^1(P, q, t), \qquad Q = q + \nabla_P S^1(P, q, t)$$

where (Hamilton–Jacobi differential equation)

$$\frac{\partial S^1(P, q, t)}{\partial t} = H\Big(P, q + \nabla_P S^1(P, q, t)\Big)$$

with $S^1(P, q, 0) = 0$.

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$$p_{n+1} = p_n - \nabla_q S^1(p_{n+1}, q_n, h), \quad q_{n+1} = q_n + \nabla_p S^1(p_{n+1}, q_n, h)$$

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$$\frac{\partial S^1(P, q, t)}{\partial t} = H\Big(P, q + \nabla_P S^1(P, q, t)\Big)$$

with $S^1(P, q, 0) = 0$. This can be formally solved:

$$S^1(P, q, h) = h\, H(P, q) + h^2 H_2(P, q) + h^3 H_3(P, q) + \dots$$

Idea of generating function integrators

$$\dot{y} = J^{-1}\nabla H(y)$$

exact solution

$$y(0), y(h), y(2h), \ldots$$

$$=$$

$$z_0,\ z_1,\ z_2,\ z_3, \ldots$$

numerical method

$$\dot{z} = J^{-1}\nabla H_h(z)$$

modified Hamiltonian

$$H_h(z) = H(z) + hH_2(z) + h^2 H_3(z) + \ldots$$

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References. Feng Kang (1986), Feng, Wu, Qin & Wang (1989), Channel & Scovel (1990), Miesbach & Pesch (1992

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Recall from

backward error analysis

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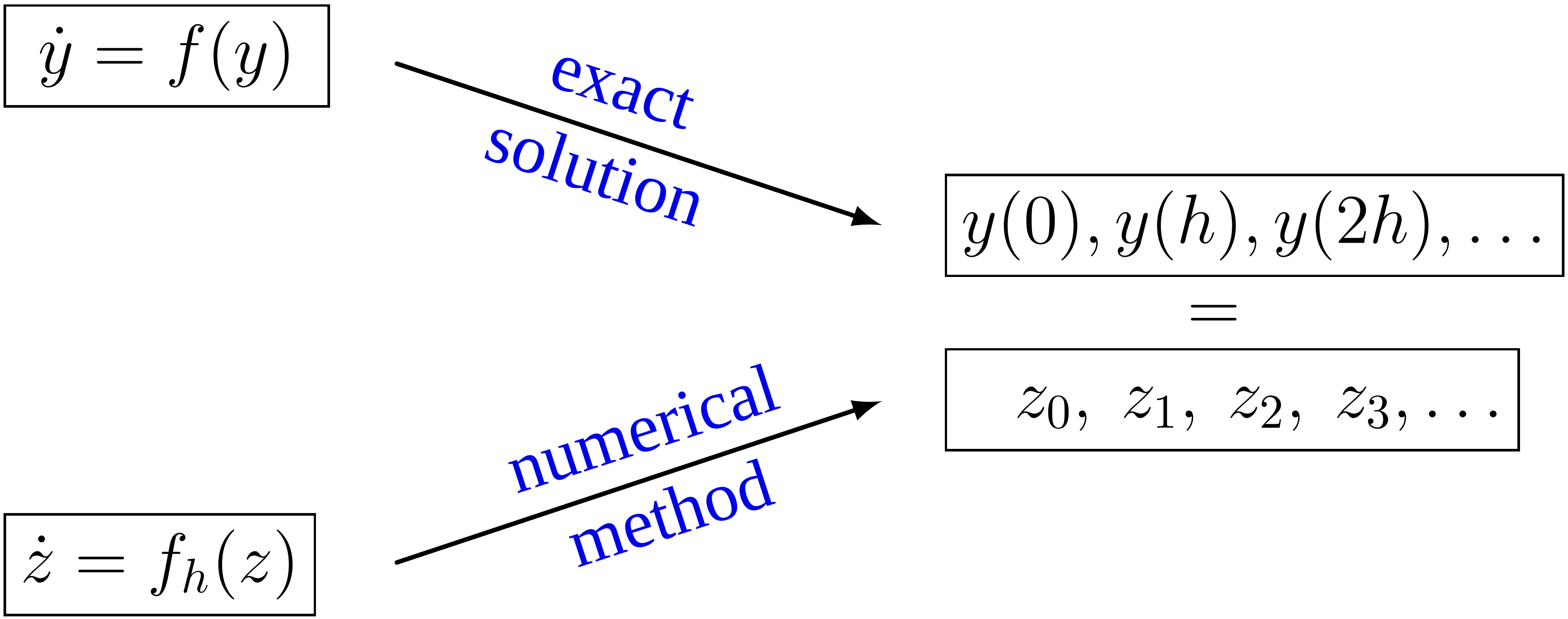
Idea of preprocessed vector field integrators



modified differential equation

$$f_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + \ldots$$

Example: implicit midpoint rule

For the general differential equation $\dot{y} = f(y)$ we consider

$$y_{n+1} = y_n + h\, f\Big(\frac{y_{n+1} + y_n}{2}\Big)$$

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Modified differential equation for the preprocessed method:

$$\dot{z} = f(z) + h^2 f_3(z) + h^4 f_5(z) + \ldots$$

where

$$\begin{aligned} f_3 &= \frac{1}{12}\Big(-f'f'f + \frac{1}{2} f''(f,f)\Big) \\ f_5 &= \frac{1}{120}\Big(f'f'f'f'f - f''(f, f'f'f) + \frac{1}{2} f''(f'f, f'f)\Big) \\ &- \frac{1}{240}\Big(\frac{1}{2} f'f'f''(f,f) - f'f''(f,f'f) - \frac{1}{2} f''(f, f''(f,f))\Big) \end{aligned}$$

Rigid body

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

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

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

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

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

Discrete Moser–Velselov (DMV) algorithm (Rattle):

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

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

The numerical solution after one step is then given by

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

Preprocessed DMV algorithm

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

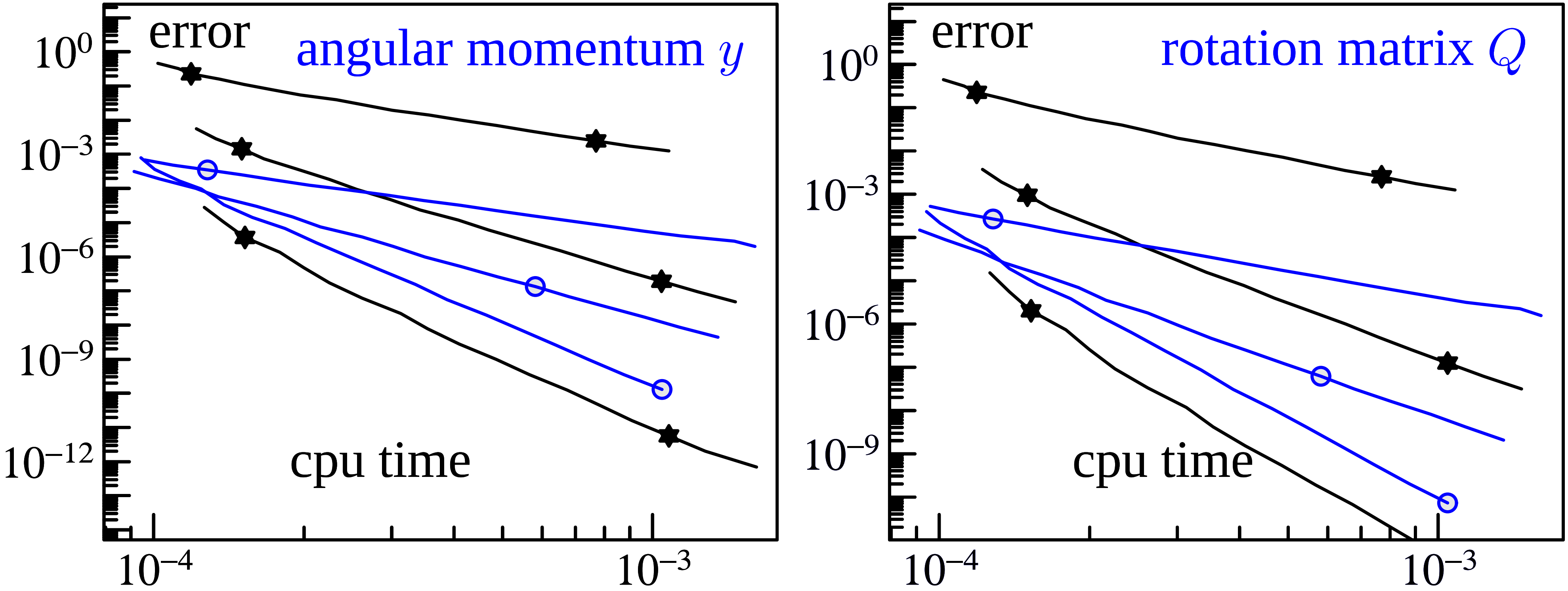
$$\frac{1}{\widetilde{I}_j} = \frac{1}{I_j}\Big(1 + h^2 s_3(y_n) + \ldots + h^{2r-2} s_{2r-1}(y_n)\Big) + h^2 d_3(y_n) + \ldots + h^{2r-2} d_{2r-1}(y_n).$$

to get an integrator of order $2r$.

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

Numerical experiment 1: asymmetric rigid body

$$I_1 = 0.6, \quad I_2 = 0.8, \quad I_3 = 1.0$$

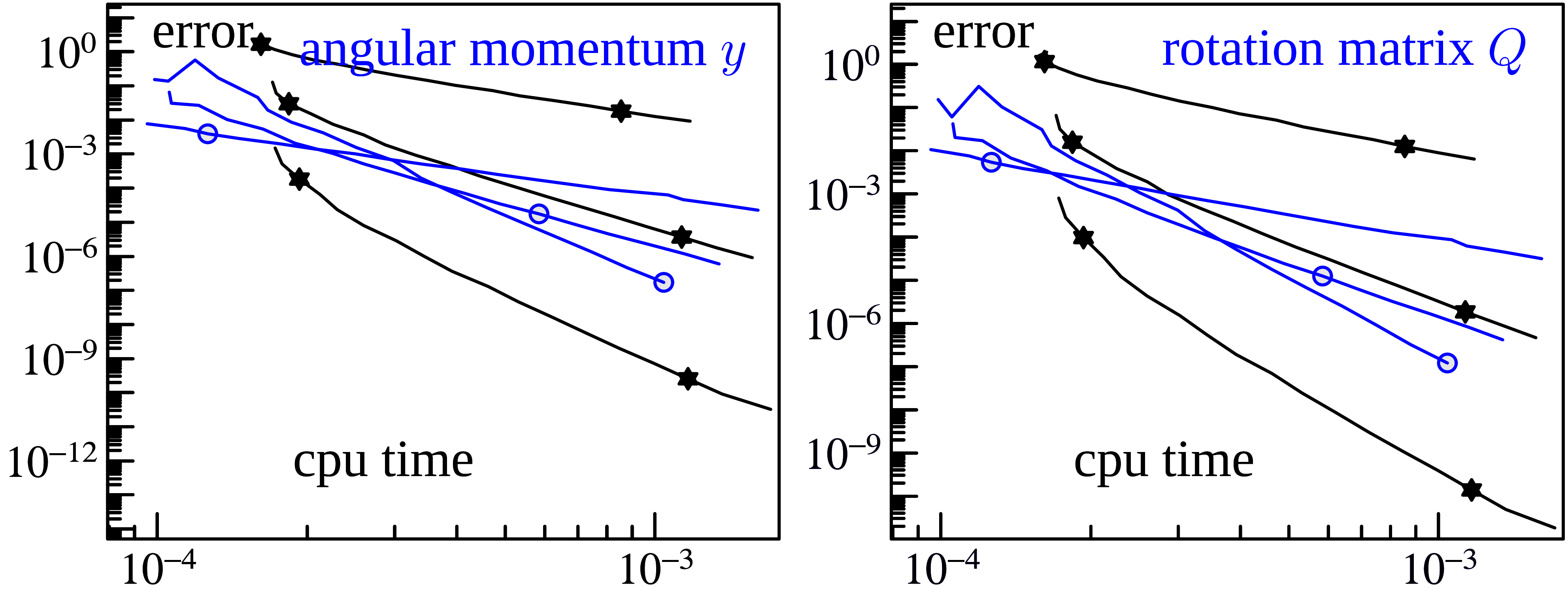


blue: splitting methods of orders 2, 4, and 6

black: preprocessed DMV of orders 2, 4, and 6

Numerical experiment 2: flat rigid body

$$I_1 = 0.345, \quad I_2 = 0.653, \quad I_3 = 1.0$$



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