Conservative, Symplectic, and Exponential Integrators

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Outline

- Symplectic Integrators
- Conservative Integrators
- Exponential Integrators
  - Robust Embedded Pairs
  - Schur Decomposition
- Conclusions

Initial Value Problems

- Given $\boldsymbol{f} : \mathbb{R}^{n+1} \to \mathbb{R}^n$, suppose $\boldsymbol{x} \in \mathbb{R}^n$ evolves according to

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, t),$$

with the initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$.

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- Hamiltonian subclass: $n = 2k$ and $\boldsymbol{x} = (\boldsymbol{q}, \boldsymbol{p})$, where $\boldsymbol{q}, \boldsymbol{p} \in \mathbb{R}^k$ satisfy

$$\frac{d\boldsymbol{q}}{dt} = \frac{\partial H}{\partial \boldsymbol{p}},$$

$$\frac{d\boldsymbol{p}}{dt} = -\frac{\partial H}{\partial \boldsymbol{q}},$$

for some function $H(\boldsymbol{q}, \boldsymbol{p}, t) : \mathbb{R}^{n+1} \to \mathbb{R}$.

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  for some function $H(\boldsymbol{q}, \boldsymbol{p}, t) : \mathbb{R}^{n+1} \to \mathbb{R}$.

- Often, the Hamiltonian H has no explicit dependence on t.

Structure-Preserving Discretizations

- Symplectic integration: conserves phase space structure of Hamilton's equations; the time step map is a canonical transformation. [Ruth 1983], [Channell & Scovel 1990], [Sanz-Serna & Calvo 1994]

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- Exponential integrators: Yield exact evolution on linear time scale

Symplectic vs. Conservative Integration

Theorem: (Ge and Marsden 1988) A C^1 symplectic map M with no explicit time-dependence will conserve a C^1 time-independent Hamiltonian $H : \mathbb{R}^n \to \mathbb{R} \iff M$ is identical to the exact evolution, up to a reparametrization of time.

Proof:

- A C^1 symplectic scheme is a canonical map M corresponding to some approximate C^1 Hamiltonian $\tilde{H}_{\tau(\boldsymbol{x},t)} : \mathbb{R}^{n+1} \to \mathbb{R}$, where the label τ denotes the time step.

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- If the mapping M does not depend explicitly on time, it can be generated by the approximate Hamiltonian $K(\boldsymbol{x}) = \tilde{H}_\tau(\boldsymbol{x}, 0)$.

- Suppose the symplectic map conserves the true Hamiltonian H:

$$0 = \frac{dH}{dt} = \frac{\partial H}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial H}{\partial p_i}\frac{dp_i}{dt} + \cancel{\frac{\partial H}{\partial t}} = [H, K],$$

where

$$[H, K] = \frac{\partial H}{\partial q_i}\frac{\partial K}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial K}{\partial q_i}.$$

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- Consequently, the trajectories in $\mathbb{R}^n$ generated by the Hamiltonians H and K coincide.

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  $\Rightarrow$ the numerical solution will *not* remain on the energy surface defined by the initial conditions!
- There exists a class of nontraditional explicit algorithms that exactly conserve nonlinear invariants to *all orders* in the time step (to machine precision).

Three-Wave Problem

- Truncated Fourier-transformed Euler equations for an inviscid 2D fluid:

$$\frac{dx_1}{dt} = f_1 = M_1 x_2 x_3,$$
$$\frac{dx_2}{dt} = f_2 = M_2 x_3 x_1,$$
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where $M_1 + M_2 + M_3 = 0$.

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where $M_1 + M_2 + M_3 = 0$.

- Then

$$\sum_k f_k x_k = 0 \Rightarrow \text{ energy } E \doteq \frac{1}{2}\sum_k x_k^2 \text{ is conserved.}$$

Secular Energy Growth

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- The Euler method

$$x_{k,i+1} = x_{k,i} + hf_k$$

yields a monotonically increasing energy:

$$\begin{aligned} E_{i+1} &= \frac{1}{2} \sum_k \left[x_k^2 + 2hf_k x_k + h^2 S_k^2 \right] \\ &= E(t) + \frac{1}{2} h^2 \sum_k S_k^2. \end{aligned}$$

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- Euler's method predicts the new energy

$$\begin{aligned} E_{i+1} &= \frac{1}{2}\sum_k \left[x_{k,i} + h(f_k + g_k)\right]^2 \\ &= E_i + \frac{1}{2}\sum_k \underbrace{\left[2hg_k x_{k,i} + h^2(f_k + g_k)^2\right]}_{\text{set to 0}}. \end{aligned}$$

- Solving for g_k yields the C–Euler discretization:

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$$\begin{aligned} x_{k,i+1} &= x_{k,i}\sqrt{1 + 2h\frac{f_k}{x_{k,i}}} \\ &= x_{k,i} + hf_k + \mathcal{O}(h^2). \end{aligned}$$

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- C–Euler is just the usual Euler algorithm applied to

$$\frac{dx_k^2}{dt} = 2f_k x_k.$$

Lemma: ([Shampine 1986]) Let $\boldsymbol{x}$ and $\boldsymbol{c}$ be vectors in $\mathbb{R}^n$. If $\boldsymbol{f} : \mathbb{R}^{n+1} \to \mathbb{R}^n$ has values orthogonal to $\boldsymbol{c}$, so that $I = \boldsymbol{c} \cdot \boldsymbol{x}$ is a linear invariant of

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, t),$$

then each stage of the explicit s-stage discretization

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_0 + h \sum_{j=0}^{i} a_{ij} \boldsymbol{f}(\boldsymbol{x}_j, t + a_i h), \qquad i = 0, \ldots, s-1,$$

also conserves I, where h is the time step and $a_{ij} \in \mathbb{R}$.

Higher-Order Conservative Integration

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- Problem: T may not be invertible!

  – Solution 1: Reduce the time step.

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- Only the final corrector stage needs to be computed in the transformed space.

Error Analysis: 1D Autonomous Case

- Exact solution (everything on RHS evaluated at x_i):

$$x_{i+1} = x_i + hf + \frac{h^2}{2} f' f + \frac{h^3}{6} (f'' f^2 + f'^2 f) + \mathcal{O}(h^4);$$

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- When $T'(x_i) \neq 0$, C–PC yields the solution

$$x_{i+1} = x_i + hf + \frac{h^2}{2} f' f + \frac{h^3}{4}\left(f'' f^2 + \frac{T'''}{3T'} f^3 \right) + \mathcal{O}(h^4),$$

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- C–PC and PC are both accurate to second order in h; for $T(x) = x^2$, they agree through third order in h.

Singular Case

- When $T'(x_i) = 0$, the conservative corrector reduces to

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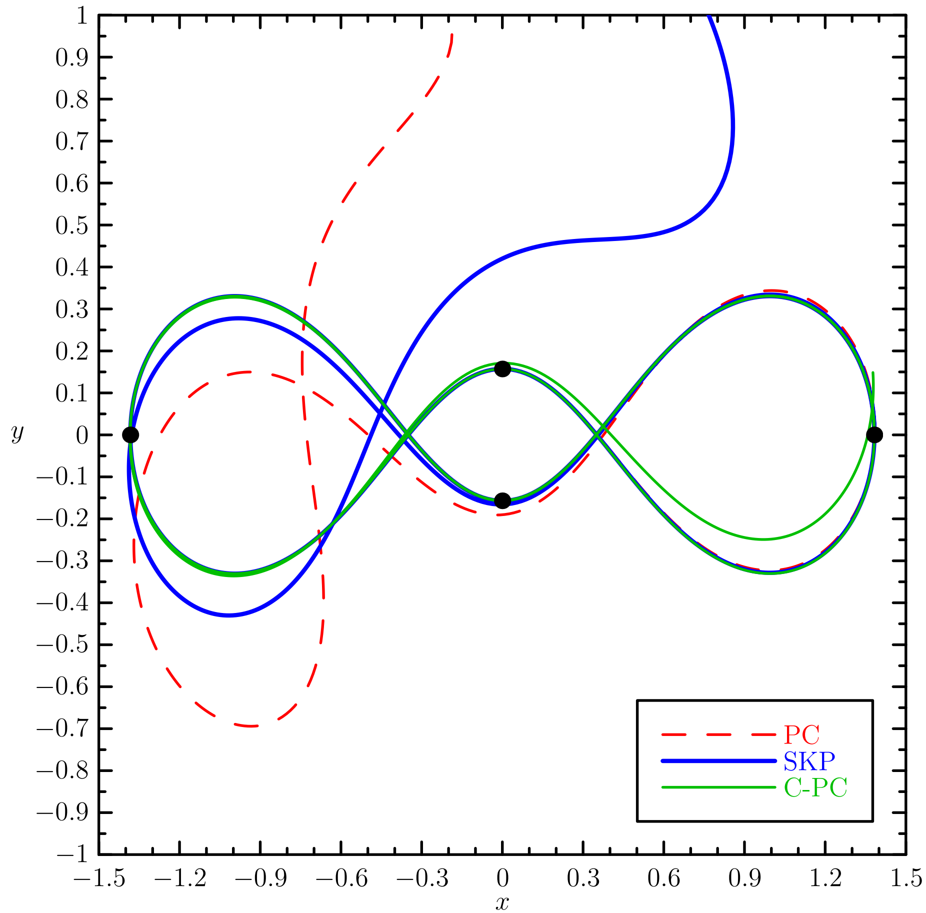
- If T and f are analytic, the existence of a solution is guaranteed as $h \to 0^+$ if the points at which T' vanishes are isolated.

Four-Body Choreography



PC, symplectic SKP, and C–PC solutions

Conservative Symplectic Integrators

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- These integrators circumvent the conditions of the Ge–Marsden theorem!

Linear Stiffness

- Consider for $y : \mathbb{R} \to \mathbb{R}$ and $L > 0$ the equation

$$\frac{dy}{dt} = -Ly,$$

with the initial condition $y(0) = y_0 \neq 0$.

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- For $hL \geq 2$, y_n does not converge to the correct steady-state solution.
- If L is large, the time step is then forced to be unreasonably small.

- This phenomenon of linear stiffness manifests itself in general driven systems of ODEs in $\mathbb{R}^n$:

$$\frac{dy}{dt} + Ly = f(y).$$

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- When the eigenvalues of L are large compared to the eigenvalues of f', a similar problem will occur.

Notation

$$\frac{dy}{dt} = f(t, y), \qquad y(0) = y_0,$$

- General s-stage Runge–Kutta scheme (scalar case):

$$y_{i+1} = y_0 + h \sum_{j=0}^{i} a_{ij} f(c_j h, y_j), \qquad i = 0, \ldots, s-1.$$

0 is the initial time; h is the time step;

y_s is the approximation to $y(h)$;

a_{ij} are the Runge–Kutta weights;

c_j are the step fractions for stage j.

Butcher Tableau ($s = 3$):

$$c_0 = 0, \qquad c_{i+1} = \sum_{j=0}^{i} a_{ij}.$$

$$\begin{array}{c|ccc} 0 & & & \\ c_1 & a_{00} & & \\ c_2 & a_{10} & a_{11} & \\ \hline 1 & a_{20} & a_{21} & a_{22} \end{array}$$

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$$\frac{d(e^{tL}y)}{dt} = e^{tL}f(y)$$

  and integrate to obtain

$$y(h) = e^{-hL}y(0) + \int_0^h e^{-(h-s)L} f(y(0+s))ds.$$

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- A quadrature rule is used to approximate the integral, while treating the exponential term exactly.

Stiff-Order Conditions

$$y_{i+1} = e^{-hL} y_0 + h \sum_{j=0}^{i} a_{ij}(-hL) f(y_j), \quad i = 0, ..., s-1.$$

- The weights a_{ij} are constructed from linear combinations of e^x and truncations of its Taylor series:

$$\varphi_0(x) = e^x$$

$$\varphi_{k+1}(x) = \frac{\varphi_k(x) - \frac{1}{k!}}{x} \quad \text{for } k \geq 0,$$

with $\varphi_k(0) = \frac{1}{k!}$.

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- Care must be exercised when evaluating φ near 0; see the C++ routines at `www.math.ualberta.ca/~bowman/phi.h`.

- A set of *stiff-order conditions* on the weights were shown by Hochbruck and Ostermann to be *sufficient* to avoid *order reduction* when L has large eigenvalues.

Exponential Euler Algorithm

$$y_{i+1} = e^{-hL} y_i + \frac{1 - e^{-hL}}{L} f(y_i),$$

- Also called Exponentially Fitted Euler, ETD Euler, filtered Euler, Lie–Euler.

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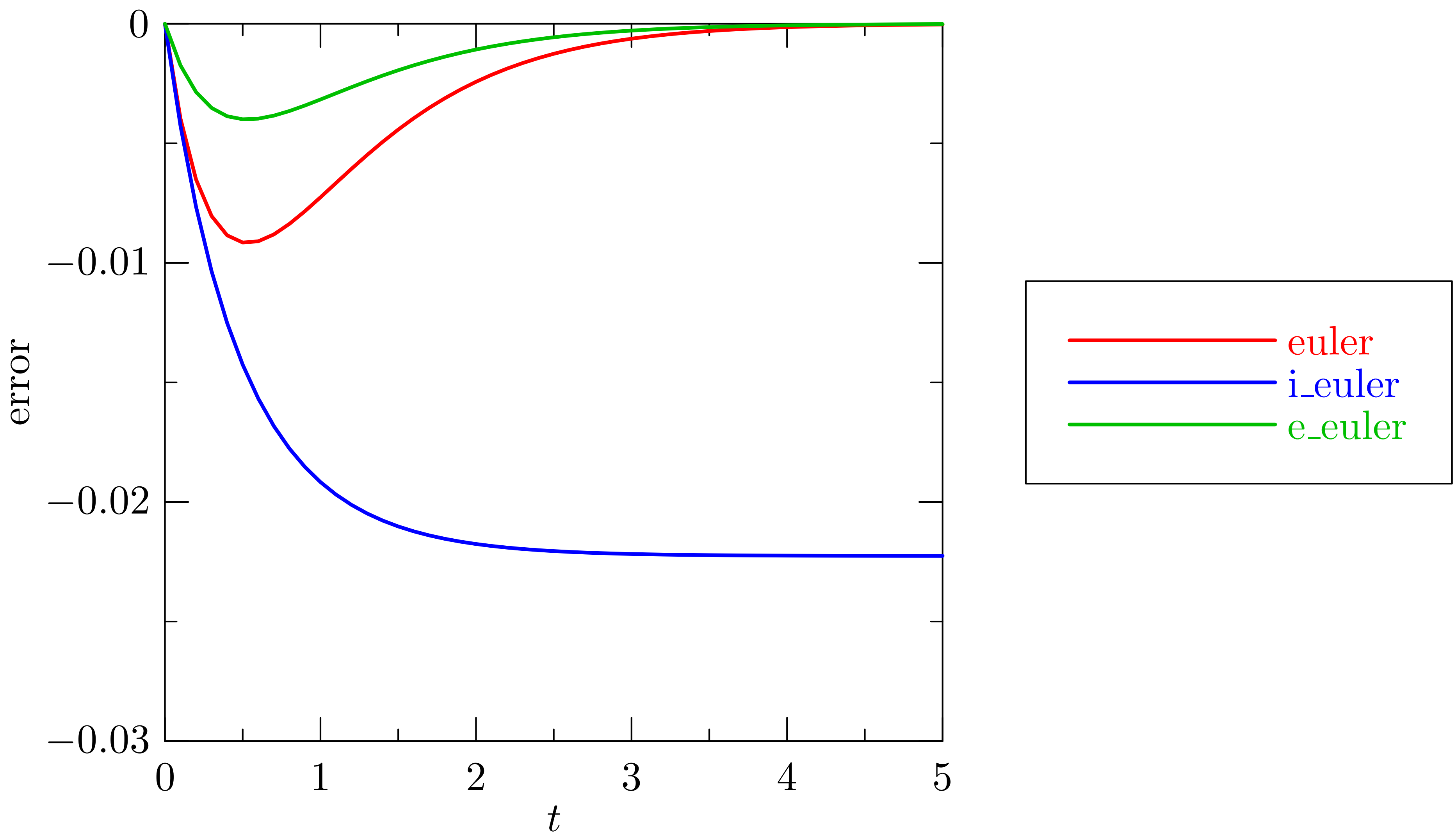
- As $h \to 0$ the Euler method is recovered:

$$y_{i+1} = y_i + hf(y_i).$$

Comparison of Euler Integrators

$$\frac{dy}{dt} + y = \cos y, \qquad y(0) = 1.$$



History of Exponential Integrators

- Certaine [1960]: Exponential Adams-Moulton
- Nørsett [1969]: Exponential Adams-Bashforth
- Verwer [1977] and van der Houwen [1977]: Exponential linear multistep method
- Friedli [1978]: Exponential Runge–Kutta
- Hochbruck *et al.* [1998]: Exponential integrators up to order 4
- Beylkin *et al.* [1998]: Exact Linear Part (ELP)
- Cox & Matthews [2002]: ETDRK3, ETDRK4; worst case: stiff order 2
- Lu [2003]: Efficient Matrix Exponential
- Hochbruck & Ostermann [2005a]: Explicit Exponential Runge–Kutta; stiff order conditions.

Embedded Pairs for Adaptive Time-Stepping

- An adaptive pair is *robust* if the order of the low-order method is never equal to the order n of the high-order method for any source function $G(t) = F(t, y(t))$ with a nonzero derivative of order less than n.

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- A nonrobust method can mislead the time step adjustment algorithm into adopting too large a time step, leading to catastrophic loss of accuracy.

(3,2) Robust Embedded Pair ERK32ZB

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_1\left(-\frac{hL}{2}\right) & & & \\
\frac{3}{4} & \frac{3}{4}\varphi_1\left(-\frac{3hL}{4}\right) - a_{11} & \frac{9}{8}\varphi_2(-\frac{3hL}{4}) + \frac{3}{8}\varphi_2(-\frac{hL}{2}) & & \\
\hline
1 & \varphi_1 - a_{21} - a_{22} - a_{23} & \frac{3}{4}\varphi_2 - \frac{1}{4}\varphi_3 & \frac{5}{6}\varphi_2 + \frac{1}{6}\varphi_3 & \\
1 & a_{30} & a_{31} & a_{32} & a_{33},
\end{array}
$$

where $\varphi_i = \varphi_i(-hL)$ and

$$
\begin{aligned}
a_{30} &= \frac{29}{18}\varphi_1 + \frac{7}{6}\varphi_1\left(-\frac{3hL}{4}\right) + \frac{9}{14}\varphi_1\left(-\frac{hL}{2}\right) + \frac{3}{4}\varphi_2 \\
&\quad + \frac{2}{7}\varphi_2\left(-\frac{3hL}{4}\right) + \frac{1}{12}\varphi_2\left(-\frac{hL}{2}\right) - \frac{8083}{420}\varphi_3 + \frac{11}{30}\varphi_3\left(-\frac{hL}{2}\right) \\
a_{31} &= -\frac{1}{9}\varphi_1 - \frac{1}{6}\varphi_1\left(-\frac{3hL}{4}\right) - \frac{1}{2}\varphi_2 \\
&\quad - \frac{1}{7}\varphi_2\left(-\frac{3hL}{4}\right) - \frac{1}{3}\varphi_2\left(-\frac{hL}{2}\right) + \frac{1}{6}\varphi_3 + \frac{1}{6}\varphi_3\left(-\frac{hL}{2}\right) \\
a_{32} &= \frac{2}{3}\varphi_1 - \frac{1}{2}\varphi_1\left(-\frac{3hL}{4}\right) - \frac{1}{7}\varphi_1\left(-\frac{hL}{2}\right) + \frac{1}{3}\varphi_2 \\
&\quad - \frac{1}{7}\varphi_2\left(-\frac{3hL}{4}\right) - \frac{1}{5}\varphi_3\left(-\frac{hL}{2}\right) \\
a_{33} &= -\frac{7}{6}\varphi_1 - \frac{1}{2}\varphi_1\left(-\frac{3hL}{4}\right) - \frac{1}{2}\varphi_1\left(-\frac{hL}{2}\right) - \frac{7}{12}\varphi_2 \\
&\quad + \frac{1}{4}\varphi_2\left(-\frac{hL}{2}\right) + \frac{2671}{140}\varphi_3 - \frac{1}{3}\varphi_3\left(-\frac{hL}{2}\right).
\end{aligned}
$$

(4,3) Robust Embedded Pair ERK43ZB

$$
\begin{array}{c|ccccc}
0 & & & & & \\
\frac{1}{6} & \frac{1}{6}\varphi_1\left(-\frac{hL}{6}\right) & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_1\left(-\frac{hL}{2}\right) - a_{11} & a_{11} & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_1\left(-\frac{hL}{2}\right) - a_{21} - a_{22} & a_{21} & a_{22} & & \\
\hline
1 & \varphi_1 - a_{31} - a_{32} - a_{33} & a_{31} & a_{32} & a_{33} & \\
1 & \varphi_1 - \frac{67}{9}\varphi_2 + \frac{52}{3}\varphi_3 & 8\varphi_2 - 24\varphi_3 & \frac{26}{3}\varphi_3 - \frac{11}{9}\varphi_2 & a_{43} & a_{44},
\end{array}
$$

where $\varphi_i = \varphi_i(-hL)$ and

$$
\begin{aligned}
a_{11} &= \frac{3}{2}\varphi_2\left(-\frac{hL}{2}\right) + \frac{1}{2}\varphi_2\left(-\frac{hL}{6}\right)\\
a_{21} &= \frac{19}{60}\varphi_1 + \frac{1}{2}\varphi_1\left(-\frac{hL}{2}\right) + \frac{1}{2}\varphi_1\left(-\frac{hL}{6}\right)\\
&\quad + 2\varphi_2\left(-\frac{hL}{2}\right) + \frac{13}{6}\varphi_2\left(-\frac{hL}{6}\right) + \frac{3}{5}\varphi_3\left(-\frac{hL}{2}\right)\\
a_{22} &= -\frac{19}{180}\varphi_1 - \frac{1}{6}\varphi_1\left(-\frac{hL}{2}\right) - \frac{1}{6}\varphi_1\left(-\frac{hL}{6}\right)\\
&\quad - \frac{1}{6}\varphi_2\left(-\frac{hL}{2}\right) + \frac{1}{9}\varphi_2\left(-\frac{hL}{6}\right) - \frac{1}{5}\varphi_3\left(-\frac{hL}{2}\right)\\
a_{33} &= \varphi_2 + \varphi_2\left(-\frac{hL}{2}\right) - 6\varphi_3 - 3\varphi_3\left(-\frac{hL}{2}\right)\\
a_{31} &= 3\varphi_2 - \frac{9}{2}\varphi_2\left(-\frac{hL}{2}\right) - \frac{5}{2}\varphi_2\left(-\frac{hL}{6}\right) + 6a_{33} + a_{21}\\
a_{32} &= 6\varphi_3 + 3\varphi_3\left(-\frac{hL}{2}\right) - 2a_{33} + a_{22}\\
a_{43} &= \frac{7}{9}\varphi_2 - \frac{10}{3}\varphi_3, \qquad a_{44} = \frac{4}{3}\varphi_3 - \frac{1}{9}\varphi_2.
\end{aligned}
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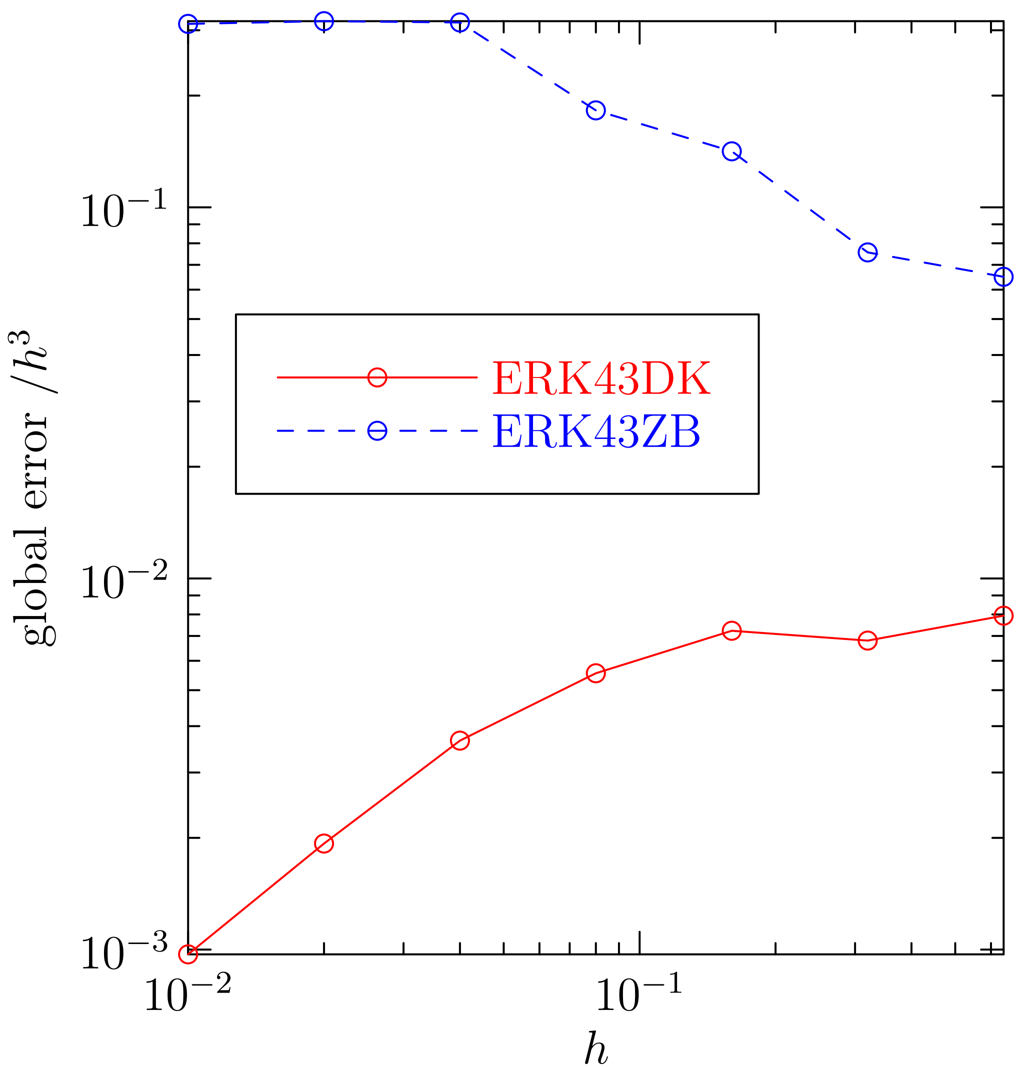
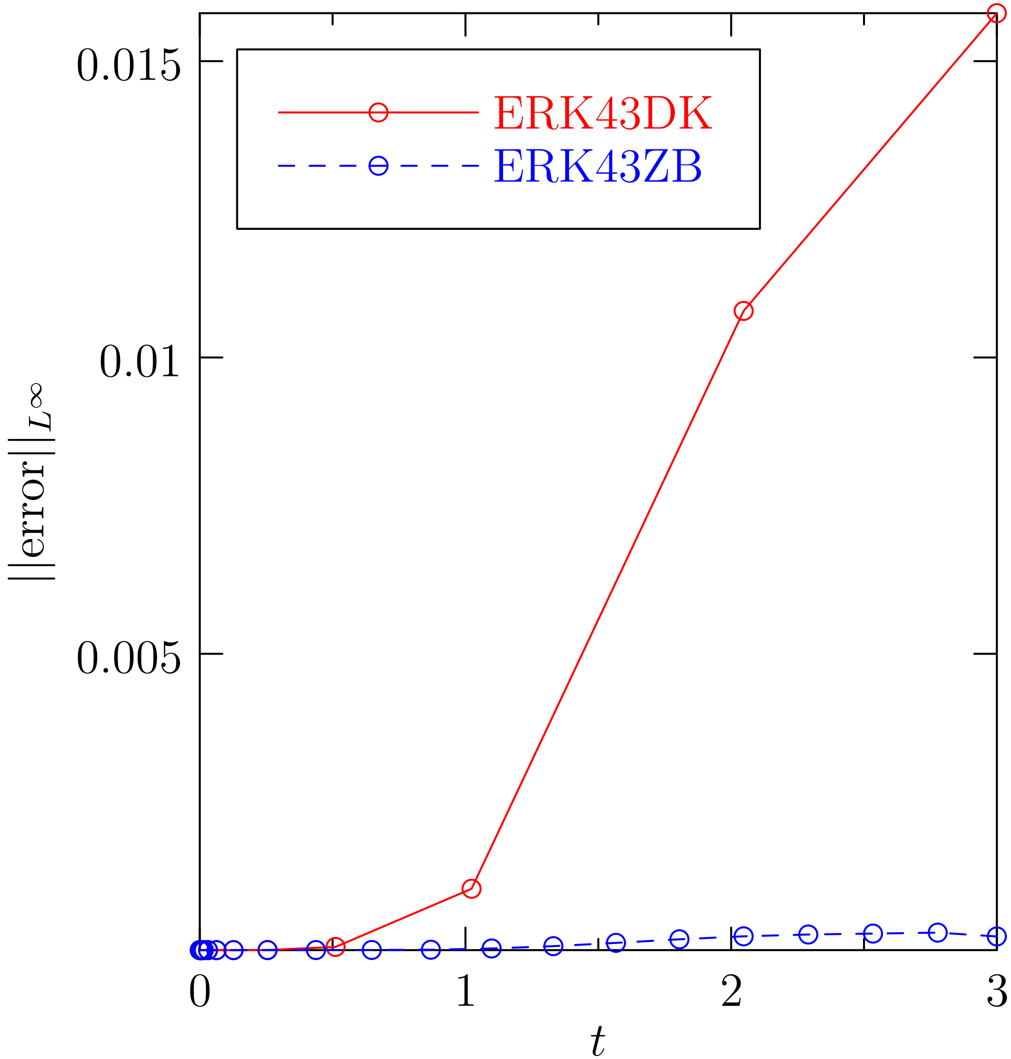
- We calculate the matrix φ_k functions with the help of Padé approximants, along with repeated scaling and squaring.

Robust vs. Non-Robust Third-Order Estimate

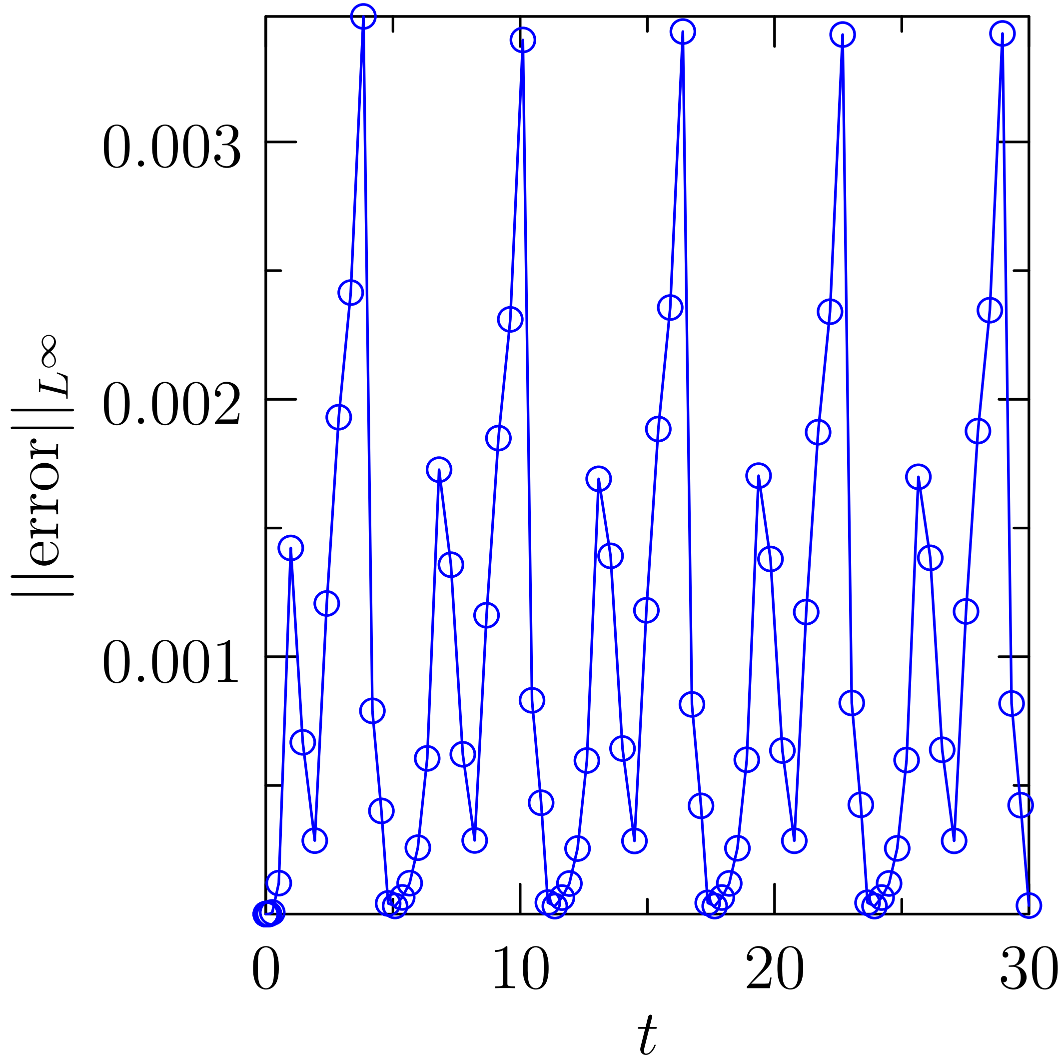


Robust vs. Non-Robust Time Evolution



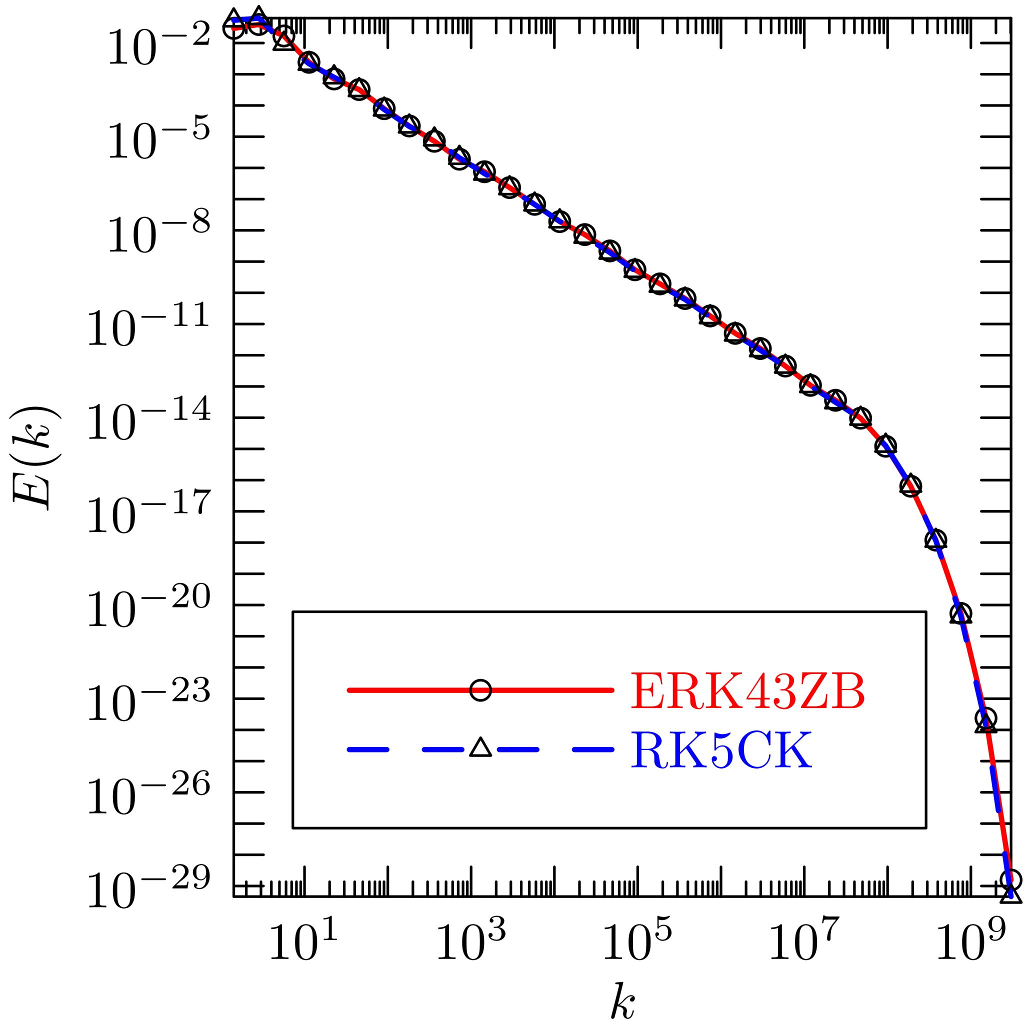
Adaptive Performance of ERK43ZB

- Choose Φ such that $y(x,t) = 10(1-x)x(1+\sin t)+2$:



GOY Shell Model of 3D Turbulence

- ERK43ZB runs over 3 times faster than the classical Cash–Karp (5,4) pair on a shell model of 3D turbulence exhibiting both linear and nonlinear stiffness:



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- We obtain

$$\frac{dy}{dt} + U(D+S)U^{\dagger}y = F(t, y).$$

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- With the optimization afforded by Schur decomposition, embedded ERK methods for step size adjustment becomes computationally viable, *even when L is a nondiagonal matrix.*
- An adaptive exponential method requires re-evaluating the φ_k functions whenever the step size is adjusted.
- However, since these are now functions of diagonal matrices, there is no longer a huge computational cost.

Claim: The term Sy does not incorporate any of the stiffness inherent in the linear term Ly.

Proof:

- On defining the integrating factor $I(t) = e^{tD}$ and $\tilde{y}(t) = I(t)y(t)$, we can transform the autonomous case to

$$\frac{d\tilde{y}}{dt} = I(t)U^{\dagger}F(UI^{-1}(t)\tilde{y}) - \tilde{S}\tilde{y},$$

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- If the stiffness only enters through the linear term Ly and not through $F(y)$, the first term on the right-hand side will not contribute any additional stiffness.

- When $F = 0$, we obtain the triangular system of equations

$$\frac{d\tilde{y}_i}{dt} = \sum_{j=i+1}^{m} \tilde{S}_{ij}\tilde{y}_j \text{ for } i = 1, \ldots, m-1 \quad \text{and} \quad \frac{d\tilde{y}_m}{dt} = 0,$$

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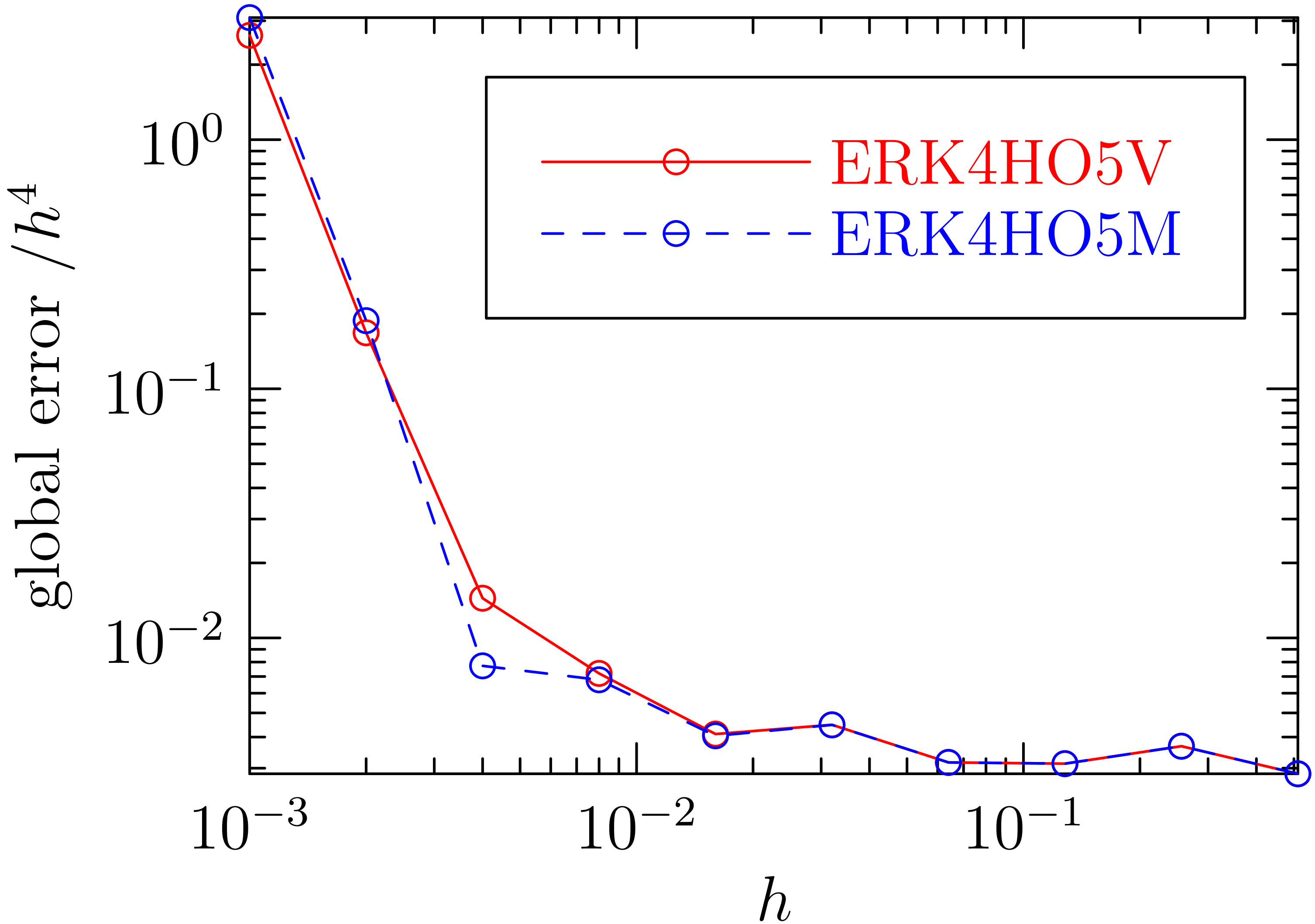
- The linear stiffness is thus *entirely contained within the diagonal term* DY.

Schur Decomposition vs. Full Solution



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- The transformation technique is relevant to integrable and nonintegrable Hamiltonian systems and even to non-Hamiltonian systems such as force-dissipative turbulence.
- Exponential integrators are explicit schemes for ODEs with a stiff linearity.
- When the nonlinear source is constant, the time-stepping algorithm is precisely the analytical solution to the corresponding first-order linear ODE.

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- New robust exponential Runge–Kutta (3,2) and (4,3) embedded pairs are well-suited to initial value problems with a dominant linearity.
- A Schur decomposition avoids the need for computing matrix exponentials, while still circumventing linear stiffness.

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