Conservative Meets Exponential: Structure-Preserving Integration Across Time Scales

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Outline

- Symplectic vs. Conservative Integration
- Conservative Integrators
- Exponential Integrators
  - Robust Embedded Pairs
- Conservative Exponential Integrators
- Conclusions

Initial Value Problems

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

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

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

- Hamiltonian subclass: $n = 2k$ and $\boldsymbol{y} = (\boldsymbol{q}, \boldsymbol{p})$, 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 $H(\boldsymbol{q}, \boldsymbol{p}, t) : \mathbb{R}^{n+1} \to \mathbb{R}$.

- 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]
- Conservative integration: conserves first integrals. [Bowman *et al.* 1997], [Shadwick *et al.* 1999], [Kotovych & Bowman 2002], [Wan *et al.* 2017]
- Positivity: preserves positive semi-definiteness of covariance matrices. [Bowman & Krommes 1997]
- Unitary integration: conserves trace of probability density matrix. [Shadwick & Buell 1997]
- 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 $\tilde{H}_\tau(\boldsymbol{y}, t) : \mathbb{R}^{n+1} \to \mathbb{R}$, where the label τ denotes the time step.
- If the mapping M does not depend explicitly on time, it can be generated by the approximate Hamiltonian $K(\boldsymbol{y}) = \tilde{H}_\tau(\boldsymbol{y}, 0)$.

- Suppose the symplectic map conserves the true Hamiltonian H:

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

where

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

- Implicit function theorem: in a neighbourhood of $\boldsymbol{y}_0 \in \mathbb{R}^n$ $\exists$ a C^1 function $\phi : \mathbb{R} \to \mathbb{R} \ni$

$$H(\boldsymbol{y}) = \phi(K(\boldsymbol{y})) \quad \text{or} \quad K(\boldsymbol{y}) = \phi(H(\boldsymbol{y})) \iff [H, K] = 0.$$

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

Conservative Integration

- Traditional numerical discretizations of nonlinear initial value problems are based on polynomial functions of the time step.
- They typically yield spurious secular drifts of nonlinear first integrals of motion (e.g. total energy).

  $\Rightarrow$ 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

- For $y = (y_1, y_2, y_3)$ and (k, j, l) cyclic $\in \{1, 2, 3\}$:

$$\frac{dy_k}{dt} + \nu y_k = f_k \doteq M_k y_j y_l.$$

  where $M_1 + M_2 + M_3 = 0$.

- When $\nu = 0$,

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

- Test parameters: $M_1 = 0.1$, $M_2 = 0.1$, $M_3 = -0.2$, initial conditions $(y_1, y_2, y_3) = (1, 0.5, 0.5)$, giving $E(0) = 0.75$.

Conservative Euler

- Euler's method yields a monotonically increasing energy:

$$E_{i+1} = E_i + \frac{1}{2}h^2 \sum_k f_k^2.$$

- Add a correction g_k to enforce exact conservation:

$$\frac{dy_k}{dt} = f_k + g_k, \qquad 2hg_k y_{k,i} + h^2(f_k + g_k)^2 = 0.$$

- Solving for g_k yields C–Euler:

$$y_{k,i+1} = \operatorname{sgn} y_{k,i+1} \sqrt{y_{k,i}^2 + 2hf_k y_{k,i}}.$$

This is just Euler's method applied to $\dfrac{dy_k^2}{dt} = 2f_k y_k$.

Higher-Order Integration

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(t, \boldsymbol{y}), \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0,$$

- General s-stage Runge–Kutta scheme:

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

h is the time step; a_{ij} are the Runge–Kutta weights;

c_j are the step fractions for stage j.

Lemma: ([Shampine 1986]) If $\boldsymbol{f}$ is orthogonal to $\boldsymbol{c}$, so that $I = \boldsymbol{c} \cdot \boldsymbol{y}$ is a linear invariant, then $\boldsymbol{y}_{i+1}$ conserves I.

Predictor–Corrector (PC)

- An explicit 2-stage Runge–Kutta scheme (Heun's method):

$$\boldsymbol{y}_0 = \boldsymbol{y}_i + h\boldsymbol{f}(\boldsymbol{y}_i, t_i), \qquad \text{Euler predictor}$$

$$\boldsymbol{y}_{i+1} = \boldsymbol{y}_i + \frac{h}{2}[\boldsymbol{f}(\boldsymbol{y}_i, t_i) + \boldsymbol{f}(\boldsymbol{y}_0, t_{i+1})], \qquad \text{trapezoidal corrector}$$

Higher-Order Conservative Integration

- Find a transformation $\boldsymbol{T}: \mathbb{R}^n \to \mathbb{R}^n$ such that the nonlinear invariants are linear functions of $\boldsymbol{\xi} = \boldsymbol{T}(\boldsymbol{y})$.
- The new value of $\boldsymbol{y}$ is then obtained by inverse transformation:

$$\boldsymbol{y}_{i+1} = \boldsymbol{T}^{-1}(\boldsymbol{\xi}_{i+1}).$$

- Problem: T may not be invertible!
  - Solution 1: Reduce the time step.
  - Solution 2: Use a traditional integrator for that time step.
  - Solution 3: Use an implicit backwards step [Shadwick & Bowman SIAM J. Appl. Math. **59**, 1112 (1999), Appendix A].
- 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 y_i):

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

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

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

  where all of the derivatives are evaluated at y_i.

- On setting $T(y) = y$, the C–PC solution reduces to the conventional PC.

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

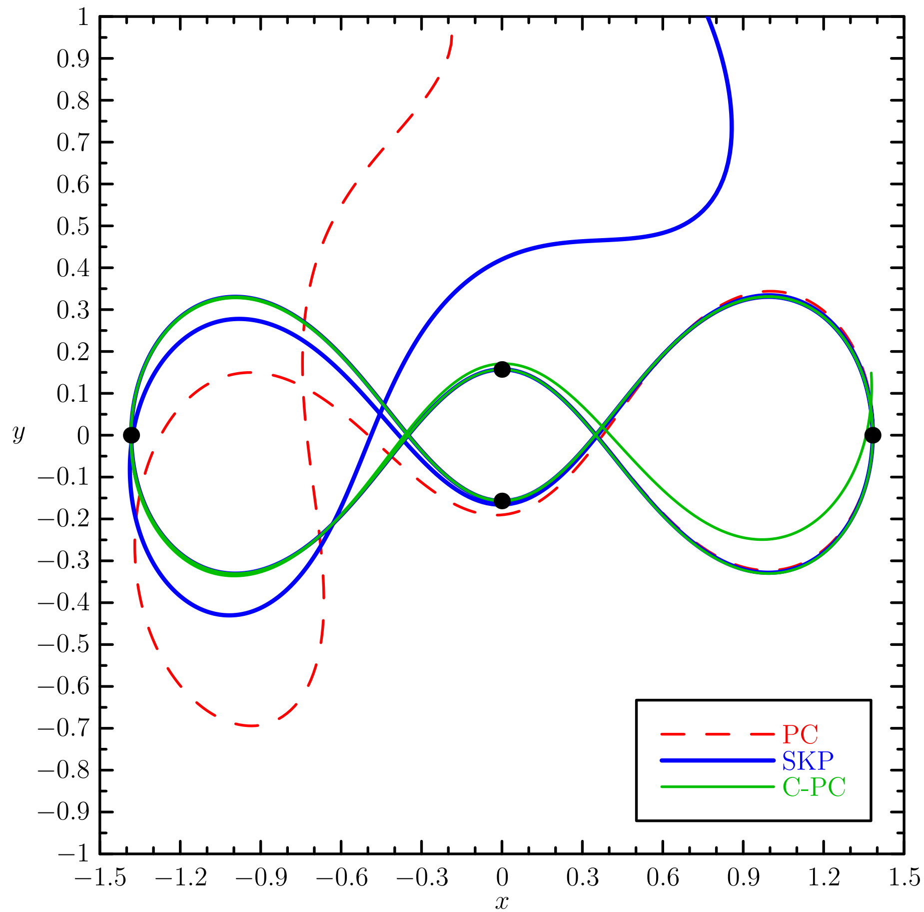
Singular Case

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

$$y_{i+1} = T^{-1}\left(T(y_i) + \frac{h}{2}T'(\tilde{y})f(\tilde{y})\right),$$

- 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

Linear Stiffness

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

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

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

- We know that the exact solution to this equation is given by

$$y(t) = y_0 e^{-tL}.$$

- Apply Euler's method with time step h:

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

- 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 $\mathbb{R}^n$:

$$\frac{d\boldsymbol{y}}{dt} + \boldsymbol{L}\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{y}).$$

- When the eigenvalues of $\boldsymbol{L}$ are large compared to those of the Jacobian of $\boldsymbol{f}$, a similar problem will occur.

Exponential Integrators

- Circumvent linear stiffness by applying a scheme that is exact on the time scale of the linear part of the problem.
- Consider

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

- Rewrite the above equation as

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

and integrate to obtain

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

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

Stiff-Order Conditions

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

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

- 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.

- If it has a fixed point, it must satisfy $y = \dfrac{f(y)}{L}$; this is then a fixed point of the ODE.

- In contrast, the popular Integrating Factor method (I-Euler).

$$y_{i+1} = e^{-hL}(y_i + hf_i)$$

  can at best have an incorrect fixed point: $y = \dfrac{hf(y)}{e^{Lh} - 1}$.

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

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

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.
- 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 $\varphi_i = \varphi_i(-hL)$.

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

(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 $\varphi_i = \varphi_i(-hL)$.

$$
\begin{aligned}
a_{11} &= \frac{3}{2}\varphi_2\left(-\frac{hL}{2}\right) + \frac{1}{2}\varphi_2\left(-\frac{hL}{6}\right) \\
a_{21} &= \frac{19}{60}\varphi_1 + \frac{1}{2}\varphi_1\left(-\frac{hL}{2}\right) + \frac{1}{2}\varphi_1\left(-\frac{hL}{6}\right) \\
&\quad + 2\varphi_2\left(-\frac{hL}{2}\right) + \frac{13}{6}\varphi_2\left(-\frac{hL}{6}\right) + \frac{3}{5}\varphi_3\left(-\frac{hL}{2}\right) \\
a_{22} &= -\frac{19}{180}\varphi_1 - \frac{1}{6}\varphi_1\left(-\frac{hL}{2}\right) - \frac{1}{6}\varphi_1\left(-\frac{hL}{6}\right) \\
&\quad - \frac{1}{6}\varphi_2\left(-\frac{hL}{2}\right) + \frac{1}{9}\varphi_2\left(-\frac{hL}{6}\right) - \frac{1}{5}\varphi_3\left(-\frac{hL}{2}\right) \\
a_{33} &= \varphi_2 + \varphi_2\left(-\frac{hL}{2}\right) - 6\varphi_3 - 3\varphi_3\left(-\frac{hL}{2}\right) \\
a_{31} &= 3\varphi_2 - \frac{9}{2}\varphi_2\left(-\frac{hL}{2}\right) - \frac{5}{2}\varphi_2\left(-\frac{hL}{6}\right) + 6a_{33} + a_{21} \\
a_{32} &= 6\varphi_3 + 3\varphi_3\left(-\frac{hL}{2}\right) - 2a_{33} + a_{22} \\
a_{43} &= \frac{7}{9}\varphi_2 - \frac{10}{3}\varphi_3, \qquad a_{44} = \frac{4}{3}\varphi_3 - \frac{1}{9}\varphi_2.
\end{aligned}
$$

Test Problem

- We illustrate robustness by comparing ERK43ZB to ERK43DK [Ding & Kang 2017] for a test problem from Hochbruck–Ostermann:

for $x \in [0,1]$ and $t \geq 0$:

$$\frac{\partial y}{\partial t}(x,t) - \frac{\partial^2 y}{\partial x^2}(x,t) = H(x,t) + \Phi(x,t).$$

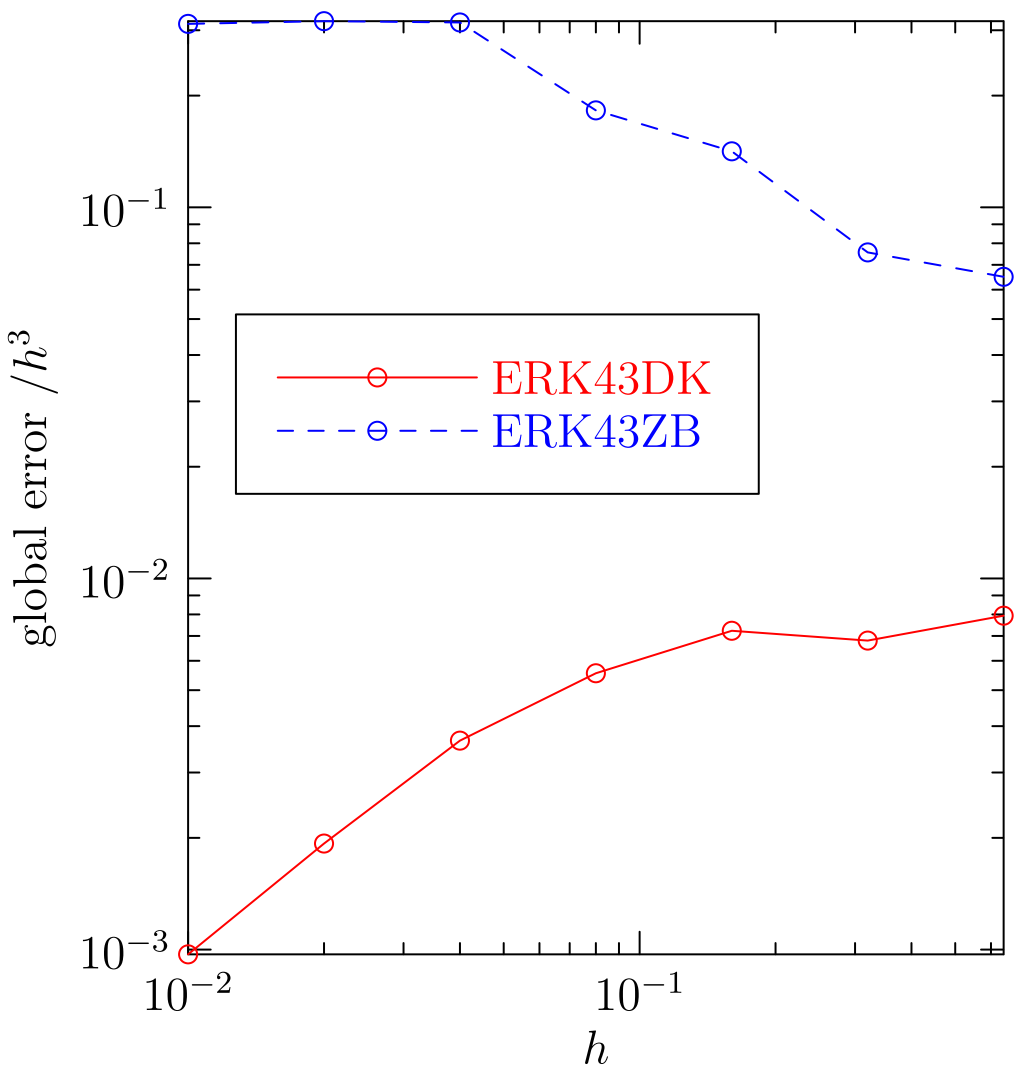
$$H(x,t) = \frac{1}{1 + y(x,t)^2}.$$

- Φ is chosen so that the exact solution is

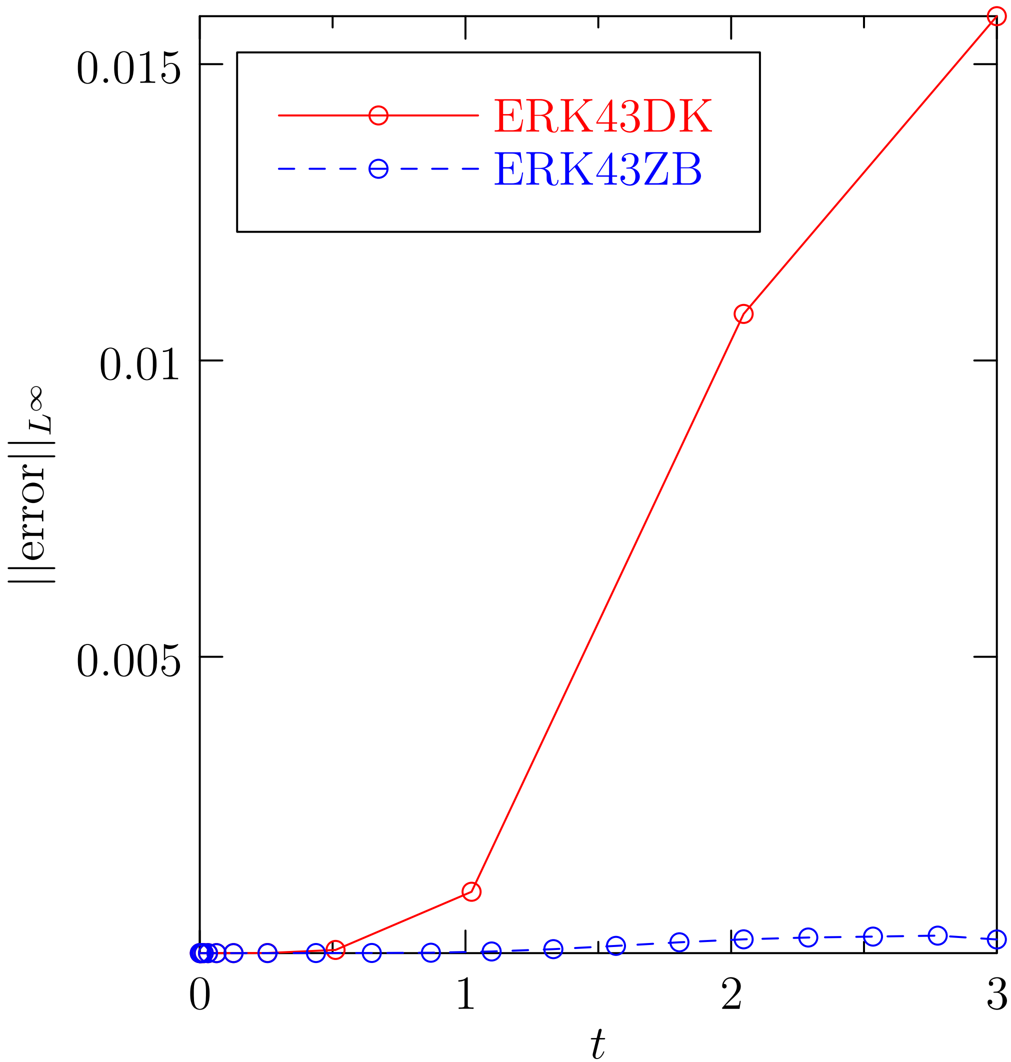
$$y(x,t) = x(1-x)e^t.$$

- 200 spatial grid points, evolve from $t = 0$ to $t = 3$.
- 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

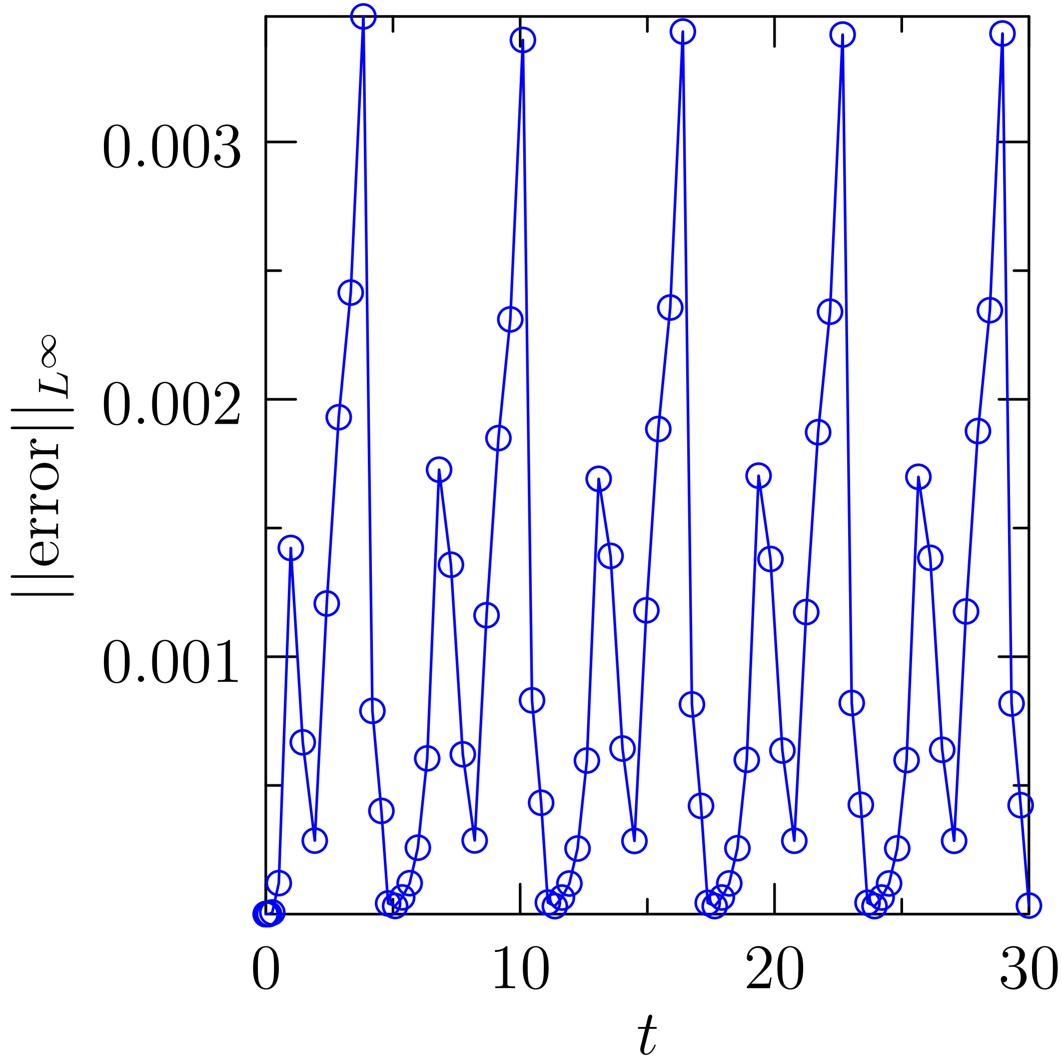


Robust vs. Non-Robust Time Evolution



Adaptive Performance of ERK43ZB

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



Conservative Exponential Integrators

- Apply the $\xi = y^2$ transformation to work in energy space:

  – Standard RK stages computed non-conservatively for predictors.

  – Final corrector uses ξ-space coefficients; transform back via $y_{n+1} = \text{sgn}(\tilde{y})\sqrt{\xi_{n+1}}$.

- When discriminant $\xi_{n+1} < 0$ (near zero crossings):

  – hybrid=0: reduce time step.

  – hybrid=1: fall back to non-conservative estimate for that mode.

CE_PC, CE_RK32ZB, CE_RK43ZB

- Three conservative exponential integrators of increasing order:

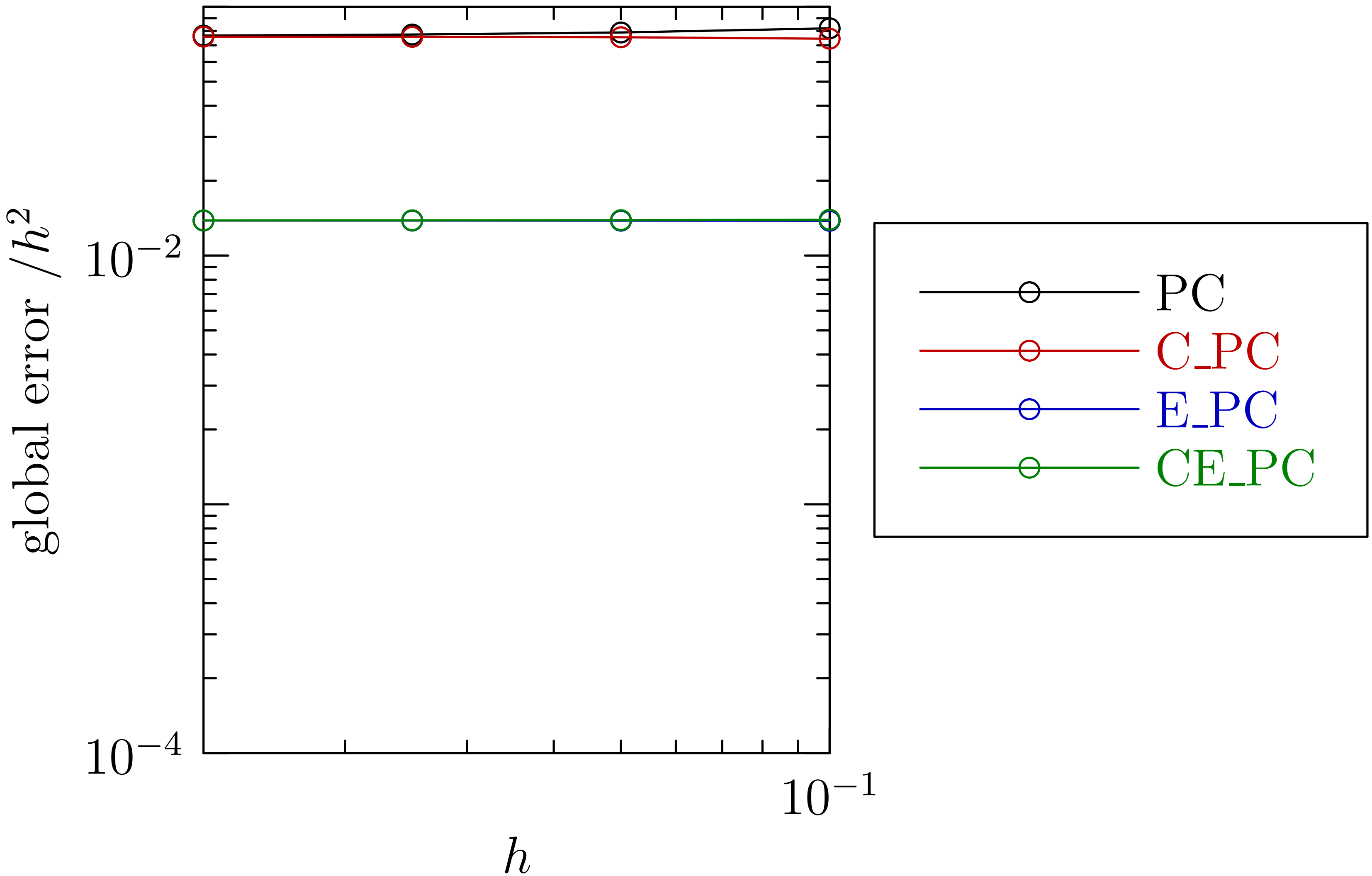
  – CE_PC: 2nd-order, embedded (2,1) pair (2 source evals/step).

  – CE_RK32ZB: 3rd-order, embedded (3,2) pair (3 source evals/step).

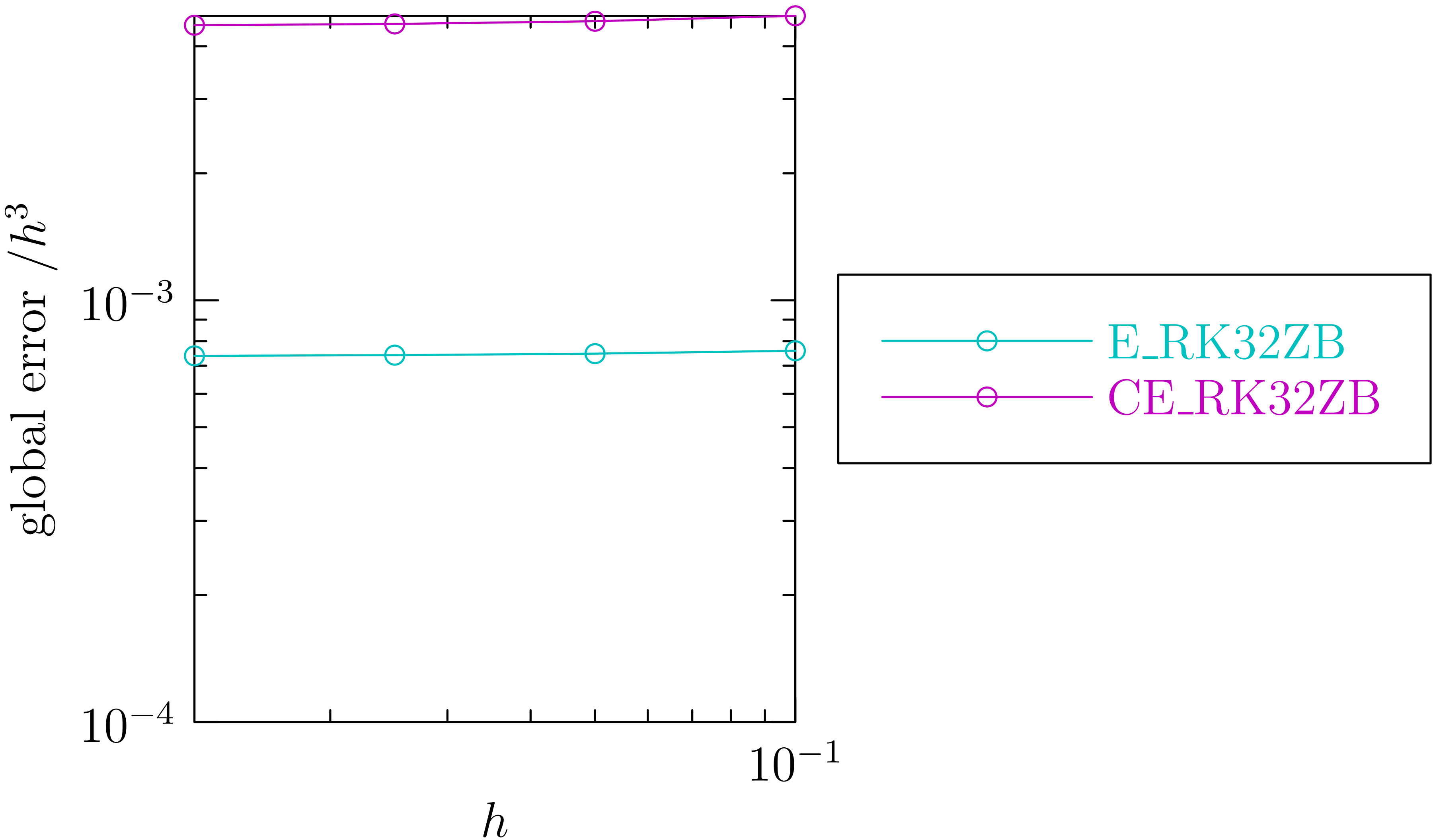
  – CE_RK43ZB: 4th-order, embedded (4,3) pair (5 source evals/step).

Convergence: CE_PC (2nd order)

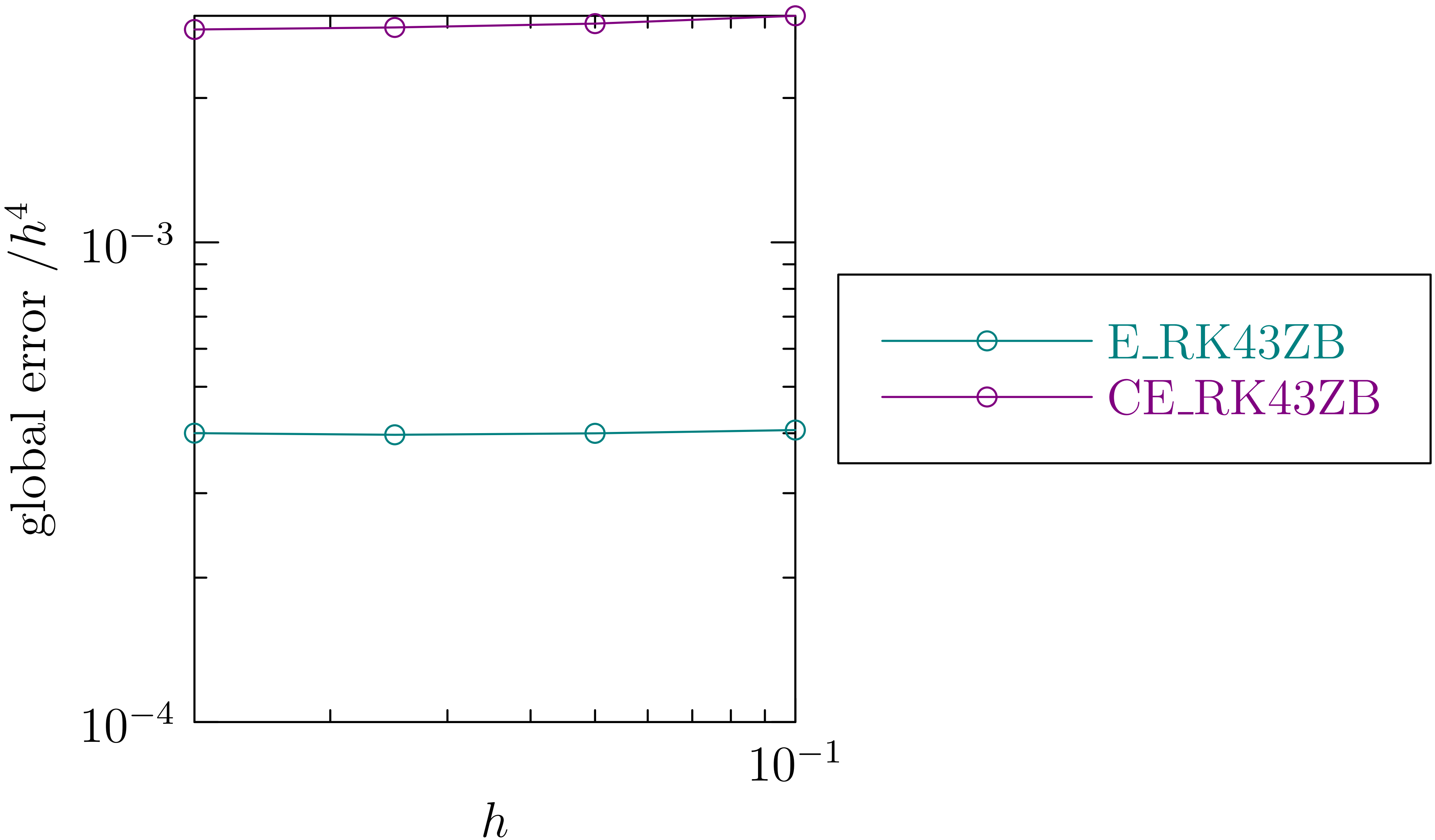
L_2 error vs. exact integrator reference.



Convergence: CE_RK32ZB (3rd order)

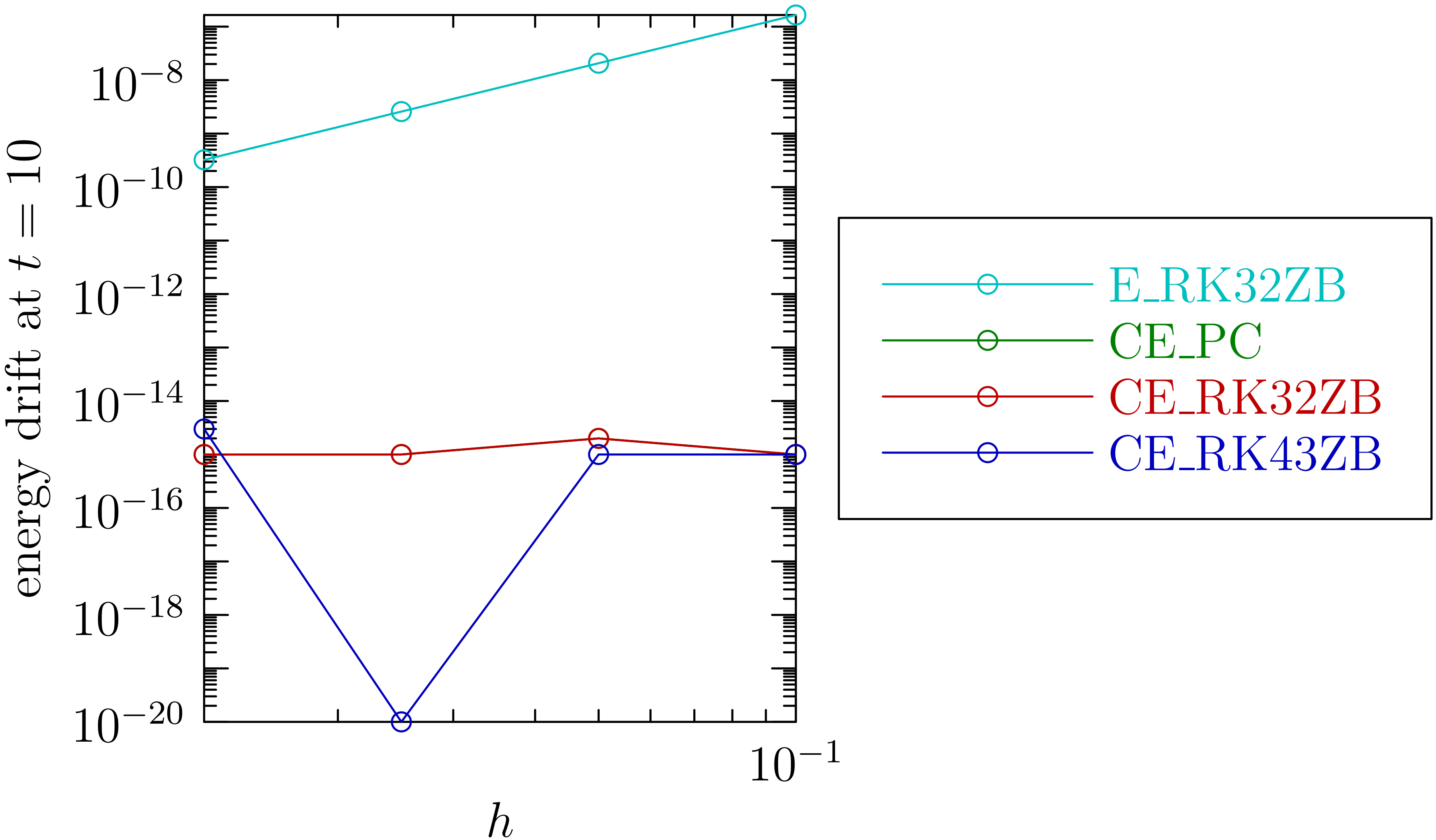


Convergence: CE_RK43ZB (4th order)



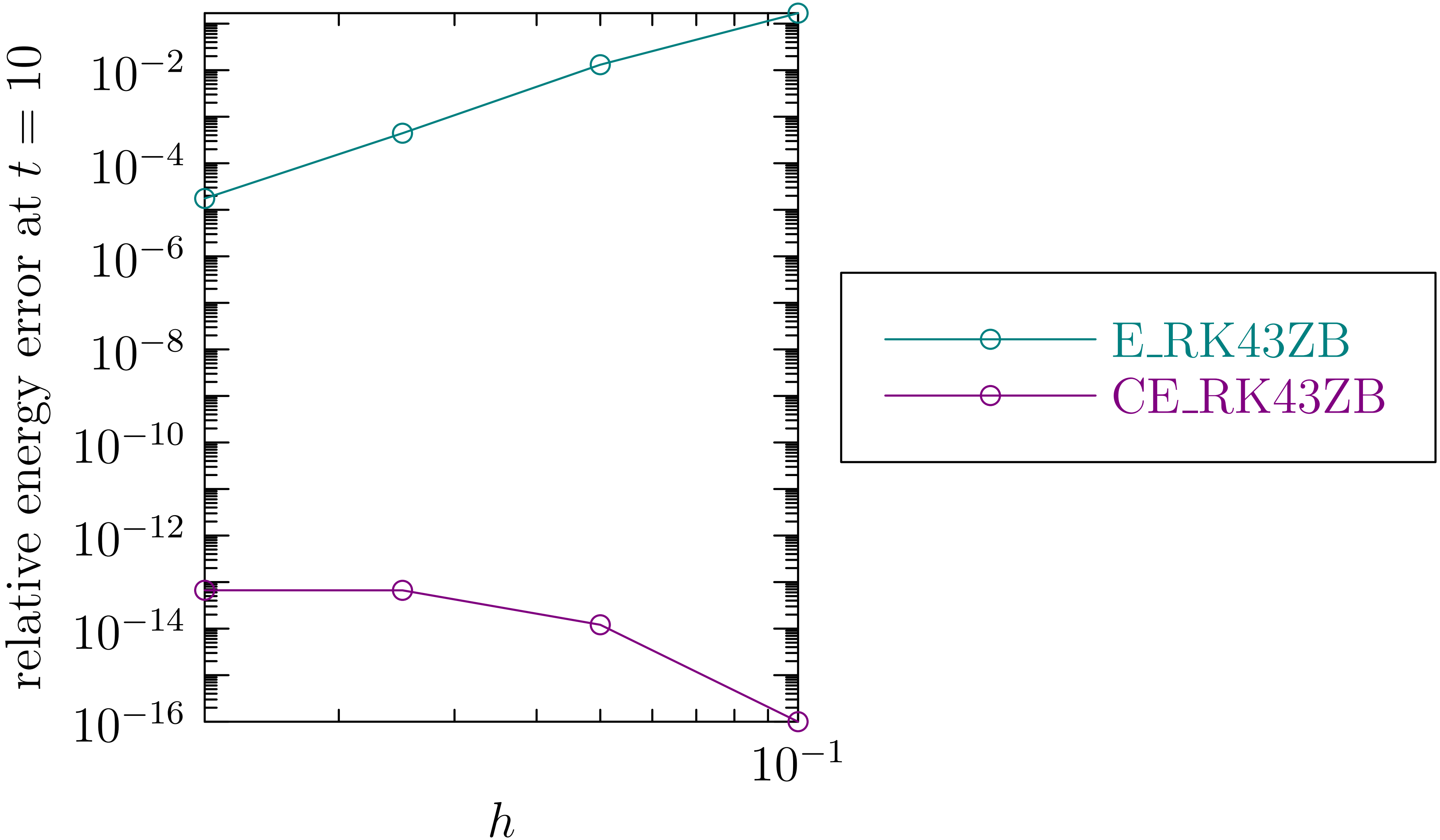
Energy Conservation: Three-Wave Problem $(\nu = 0)$

Exact $E(t) = E(0) = 0.75$



Growing Solution: Three-Wave Problem $(\nu = -0.5)$

Exact $E(10) = 0.75\, e^{10}$



Conclusions

- Numerical discretizations that preserve physically relevant structure or known analytic properties are desirable.
- Traditional numerical discretizations of conservative systems generically yield artificial secular drifts of nonlinear invariants.
- New exactly conservative but explicit integration algorithms have been developed.
- 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.

- Unlike integrating factor methods, exponential integrators have the correct fixed point behaviour.
- We derived adaptive ERK pairs by symbolically solving the Hochbruck–Ostermann stiff-order conditions.
- A key requirement is that the pair be robust: if the nonlinear source function has nonzero total time derivatives, the order of the low-order estimate should never exceed its design value.
- New robust exponential Runge–Kutta (3,2) and (4,3) embedded pairs are well-suited to initial value problems with a dominant linearity.
- Conservative exponential integrators combine both approaches: they preserve nonlinear first integrals to machine precision while circumventing linear stiffness.

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