Exponential Integrators

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Notation

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

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

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

0 is the initial time; τ is the time step;

y_s is the approximation to $y(\tau)$;

a_{ij} are the Runge–Kutta weights;

c_j are the step fractions for stage j.

Butcher Tableau ($s = 3$):

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

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

Motivation

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

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

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

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

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

- Apply Euler's method with time step τ:

$$y_{n+1} = (1 - \tau L) y_n.$$

- For $\tau L \geq 2$, y_n does not converge to the steady state: if L is too large, the time step is forced to be unreasonably small.

- This phenomenon of linear stiffness manifests itself in more general systems of ODEs, when $\boldsymbol{y}(t) \in \mathbb{R}^n$,

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

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

Exponential Integrators

- We remedy the problem of stiffness by applying a scheme that is exact on the time scale of the linear part of the problem. We call all such schemes exponential integrators.

- Consider

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

- Goal: Solve on the linear time scale exactly; avoid the linear time-step restriction $\tau L \ll 1$.

- Rewrite the above equation as

$$\frac{d(e^{\mathbf{L}t}\boldsymbol{y})}{dt} = e^{\mathbf{L}t}\boldsymbol{f}(\boldsymbol{y}).$$

Time-domain approach

- There are two ways to proceed from here. The first involves integrating and applying a quadrature rule:

$$\boldsymbol{y}(\tau) = e^{-\tau \mathbf{L}}\boldsymbol{y}(0) + \int_0^{\tau} e^{-(\tau-s)\mathbf{L}} \boldsymbol{f}(\boldsymbol{y}(0+s))ds.$$

- The idea is to apply a quadrature rule that approximates $\boldsymbol{f}$ but treats the exponential term exactly. This approach gives rise to the discretization

$$\boldsymbol{y}_{i+1} = e^{-\tau \mathbf{L}}\boldsymbol{y}_0 + \tau \sum_{j=0}^{i} \mathbf{a}_{ij}(-\tau \mathbf{L})\boldsymbol{f}(\boldsymbol{y}_j),$$

  where $i = 0, ..., s-1$.

- The weights $\mathbf{a}_{ij}$ are constructed from linear combinations of $e^{-\tau \mathbf{L}}$ and truncations of its Taylor series.

- The weights are determined by a set of *stiff order conditions*.

Exponential Euler Algorithm (E-Euler)

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

- Also called Exponentially Fitted Euler, ETD Euler, filtered Euler, Lie–Euler.
- As $\tau \to 0$ the Euler method is recovered:

$$y_{i+1} = y_i + \tau f(y_i).$$

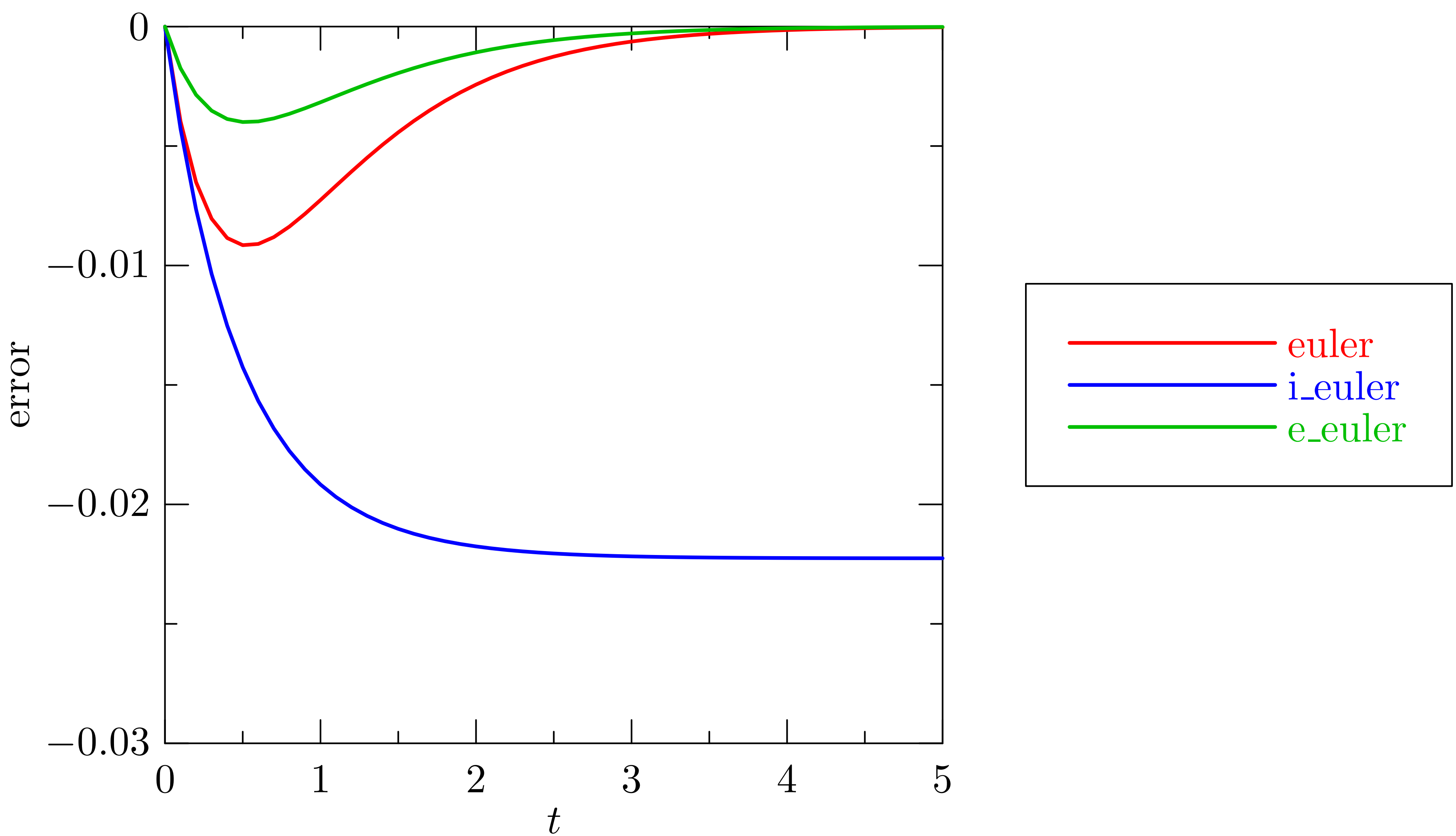
- If E-Euler has a fixed point, it must satisfy $y = \frac{f(y)}{L}$; this is then a fixed point of the ODE.
- In contrast, the popular Integrating Factor method (I-Euler).

$$y_{i+1} = e^{-\tau L}(y_i + \tau f_i)$$

can at best have an incorrect fixed point: $y = \frac{\tau f(y)}{e^{L\tau} - 1}$.

Comparison of Euler Integrators

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



History

- 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.

Bogacki–Shampine (3,2) Pair (RK3-BS)

- Embedded 4-stage pair [Bogacki & Shampine 1989]:

$$
\begin{array}{c|cccc}
0 & \frac{1}{2} & & & \\[2ex]
\frac{1}{2} & 0 & \frac{3}{4} & & \\[2ex]
\frac{3}{4} & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} & \\[2ex]
\hline
1 & \frac{7}{24} & \frac{1}{4} & \frac{1}{3} & \frac{1}{8}
\end{array}
\qquad
\begin{array}{l}
\\[2ex] \\[2ex]
\longleftarrow \text{3rd order} \\[2ex]
\longleftarrow \text{2nd order}
\end{array}
$$

Embedded (3,2) Exponential Pair (ERK3-HO)

[Bowman *et al.* 2006]

- Let $\boldsymbol{x} = -\mathsf{L}\tau$ and $\varphi_2(\boldsymbol{x}) = \boldsymbol{x}^{-2}(e^{\boldsymbol{x}} - \mathbf{1} - \boldsymbol{x})$:

$$\boldsymbol{a}_{00} = \frac{1}{2}\varphi\left(\frac{1}{2}\boldsymbol{x}\right),$$

$$\boldsymbol{a}_{10} = \frac{3}{4}\varphi\left(\frac{3}{4}\boldsymbol{x}\right) - \boldsymbol{a}_{11},\ \ \boldsymbol{a}_{11} = \frac{9}{8}\varphi_2\left(\frac{3}{4}\boldsymbol{x}\right) + \frac{3}{8}\varphi_2\left(\frac{1}{2}\boldsymbol{x}\right),$$

$$\boldsymbol{a}_{20} = \varphi(\boldsymbol{x}) - \boldsymbol{a}_{21} - \boldsymbol{a}_{22},\ \ \boldsymbol{a}_{21} = \frac{1}{3}\varphi(\boldsymbol{x}), \boldsymbol{a}_{22} = \frac{4}{3}\varphi_2(\boldsymbol{x}) - \frac{2}{9}\varphi(\boldsymbol{x}),$$

$$\boldsymbol{a}_{30} = \varphi(\boldsymbol{x}) - \frac{17}{12}\varphi_2(\boldsymbol{x}),\ \ \boldsymbol{a}_{31} = \frac{1}{2}\varphi_2(\boldsymbol{x}),\ \ \boldsymbol{a}_{32} = \frac{2}{3}\varphi_2(\boldsymbol{x}),\ \ \boldsymbol{a}_{33} = \frac{1}{4}\varphi_2(\boldsymbol{x}).$$

- $\boldsymbol{y}_3$ has stiff order 3 [Hochbruck and Ostermann 2005].
- $\boldsymbol{y}_4$ provides a second-order estimate for adjusting the time step.
- $\mathsf{L} \to \mathbf{0}$: reduces to [3,2] Bogacki–Shampine Runge–Kutta pair.

Exponential domain approach

- We now present a different way to view exponential integrators.
- To illustrate the main idea, we first consider the scalar variant, where $y : \mathbb{R} \to \mathbb{R}$:

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

- It is convenient to let $g(t) = f(y(t))$, introduce the integrating factor

$$I(t) = e^{Lt},$$

and define $Y(t) = I(t)y(t)$, so that

$$\frac{dY}{dt} = Ig.$$

- Discretization should be performed in the (I, Y) space instead of the (t, y) space!

- We perform the change of variable $dt\, I = L^{-1} dI$:

$$\frac{dY}{dI} = \frac{1}{L} g(t(I)),$$

where $t(I) = \frac{1}{L} \log I$.

- If g is analytic, we can expand it in a Taylor series

$$g(t) = \sum_{k=0}^{\infty} g^{(k)}(0) \frac{t^k}{k!}.$$

- This allows us to integrate dY/dI over I to obtain the exact solution

$$Y = Y_0 + \frac{1}{L} \sum_{k=0}^{\infty} g^{(k)}(0) \frac{1}{k!} \int_1^I (\log \bar{I})^k \, d\bar{I}.$$

- On inspecting the classical Runge–Kutta discretization of the transformed equation $dY/dI = g/L$, it is possible to obtain corresponding finite difference approximations of the derivatives $g^{(k)}(0)$ in terms of the Runge-Kutta sampled function values.

- If we inductively define

$$\varphi_0(x) = e^x$$
$$\varphi_{k+1}(x) = \frac{\varphi_k(x) - \frac{1}{k!}}{x} \quad \text{for } k \geq 0,$$

with $\varphi_k(0) = \frac{1}{k!}$, the exact solution becomes

$$y = I^{-1}y_0 + \sum_{k=0}^{\infty} g^{(k)}(0)\varphi_{k+1}(-L\tau)\tau^{k+1},$$

where τ is a single time step.

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

General third-order RK scheme

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

- Let $g(t) = f(t, y(t)) = a + bt + ct^2 + \mathcal{O}(t^3)$.
- Given two distinct step fractions c_1 and c_2, use the classical order conditions to compute the weights a_{ij}:

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

- A key ingredient is the Vandermonde matrix:

$$\boldsymbol{V} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & c_1 & c_2 \\ 0 & c_1^2 & c_2^2 \end{bmatrix},$$

which is used to compute the last row of the tableau:

$$\begin{bmatrix} a_{20} \\ a_{21} \\ a_{22} \end{bmatrix} = \boldsymbol{V}^{-1} \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \end{bmatrix} = \begin{bmatrix} \dfrac{2-3c_1}{6c_1c_2} - \dfrac{1}{2c_1} + 1 \\ \dfrac{2-3c_1}{6c_1(c_1-c_2)} + \dfrac{1}{2c_1} \\ \dfrac{2-3c_1}{6c_2(c_2-c_1)} \end{bmatrix},$$

as well as finite-difference weights for approximating derivatives of g, such as

$$\tau g'(0) \approx -\frac{1}{c_1} g_0 + \frac{1}{c_1} g_1$$
$$\tau^2 g''(0) \approx \frac{2}{c_1 c_2} g_0 + \frac{2}{c_1(c_1-c_2)} g_1 + \frac{2}{c_2(c_2-c_1)} g_3,$$

where $g_i = g(c_i\tau) = a + bc_i\tau + cc_i^2\tau^2$.

- We use these results to rewrite the final stage of RK3:

$$y_3 = y_0 + \tau g(0) + \tau^2 g'(0)/2 + \tau^3 g''(0)/6.$$

General third-order ERK scheme

- Letting $x = -L\tau$, we obtain the ERK3 integrator:

$$
\begin{aligned}
y_1 &= y_0\varphi_0(c_1x) + c_1\tau g_0\varphi_1(c_1x),\\
y_2 &= y_0\varphi_0(c_2x) + c_2\tau g_0\varphi_1(c_2x) + 2a_{11}\tau(g_1 - g_0)\varphi_2(c_2x),\\
y_3 &= y_0\varphi_0(x) + \tau g_0\varphi_1(x) + \frac{1}{c_1}\tau(g_1 - g_0)\varphi_2(x) +\\
&\quad (2-3c_1)\tau\left(\frac{1}{c_1c_2}g_0 + \frac{1}{c_1(c_1-c_2)}g_1 + \frac{1}{c_2(c_2-c_1)}g_2\right)\varphi_3(x).
\end{aligned}
$$

ERK-BS(3,2) integrator with 4 stages

- Let $x = -L\tau$.

$$a_{00} = \frac{1}{2}\varphi_1\left(\frac{1}{2}x\right),$$

$$a_{10} = \frac{3}{4}\varphi_1\left(\frac{3}{4}x\right) - \frac{3}{2}\varphi_2\left(\frac{3}{4}x\right), \qquad a_{11} = \frac{3}{2}\varphi_2\left(\frac{3}{4}x\right),$$

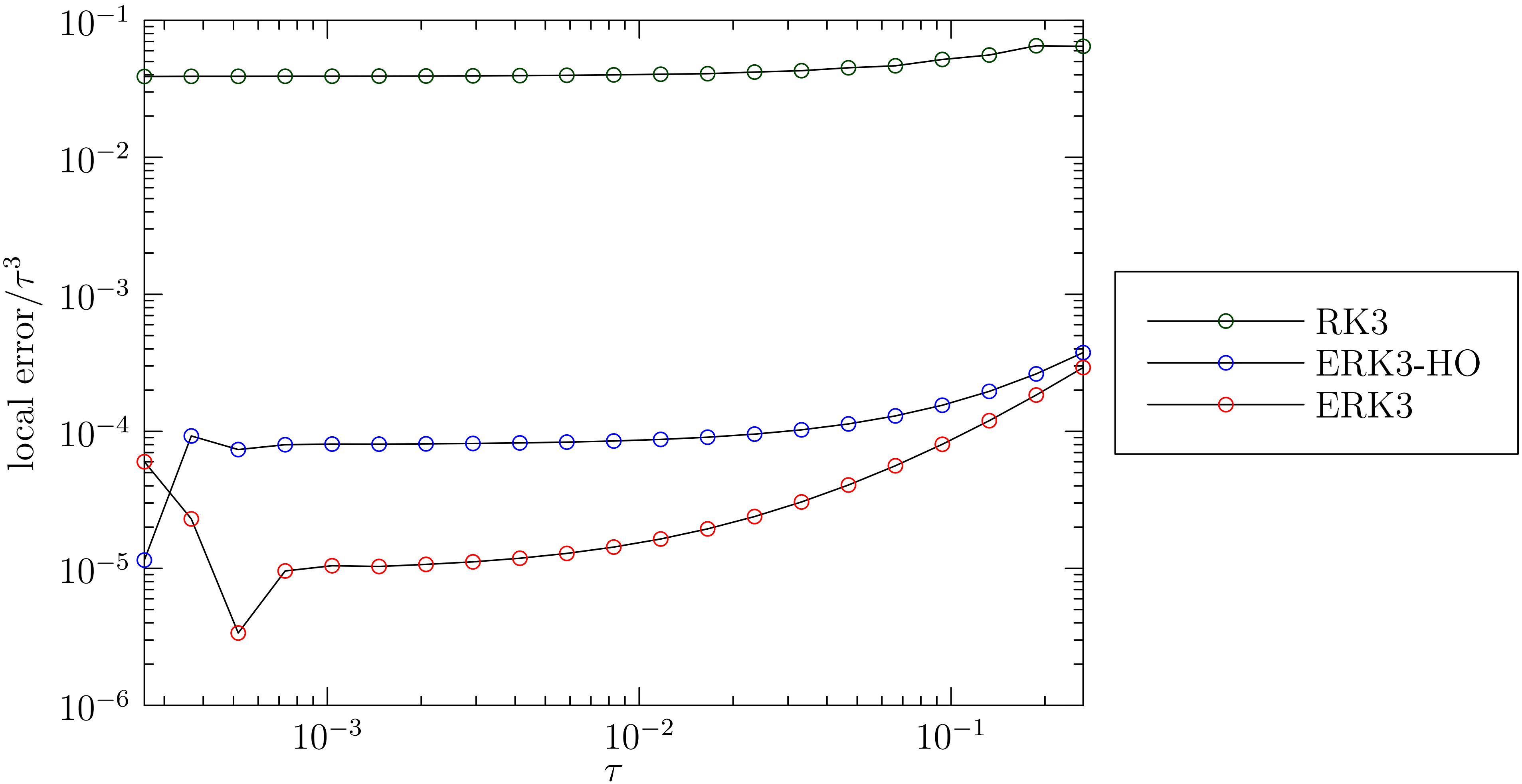
$$a_{20} = \varphi_1(x) - 2\varphi_2(x) + \frac{4}{3}\varphi_3(x), \quad a_{21} = 2\varphi_2(x) - 4\varphi_3(x), \quad a_{22} = \frac{8}{3}\varphi_3(x),$$

$$a_{30} = \varphi_1(x) - \frac{17}{12}\varphi_2(x), \qquad a_{31} = \frac{1}{2}\varphi_2(x), \qquad a_{32} = \frac{2}{3}\varphi_2(x),$$

$$a_{33} = \frac{1}{4}\varphi_2(x).$$

Third-order integration test:

$$\frac{dy}{dt} + 4y = y^2 \sin y \qquad y(0) = 1, \qquad t = 1.5$$



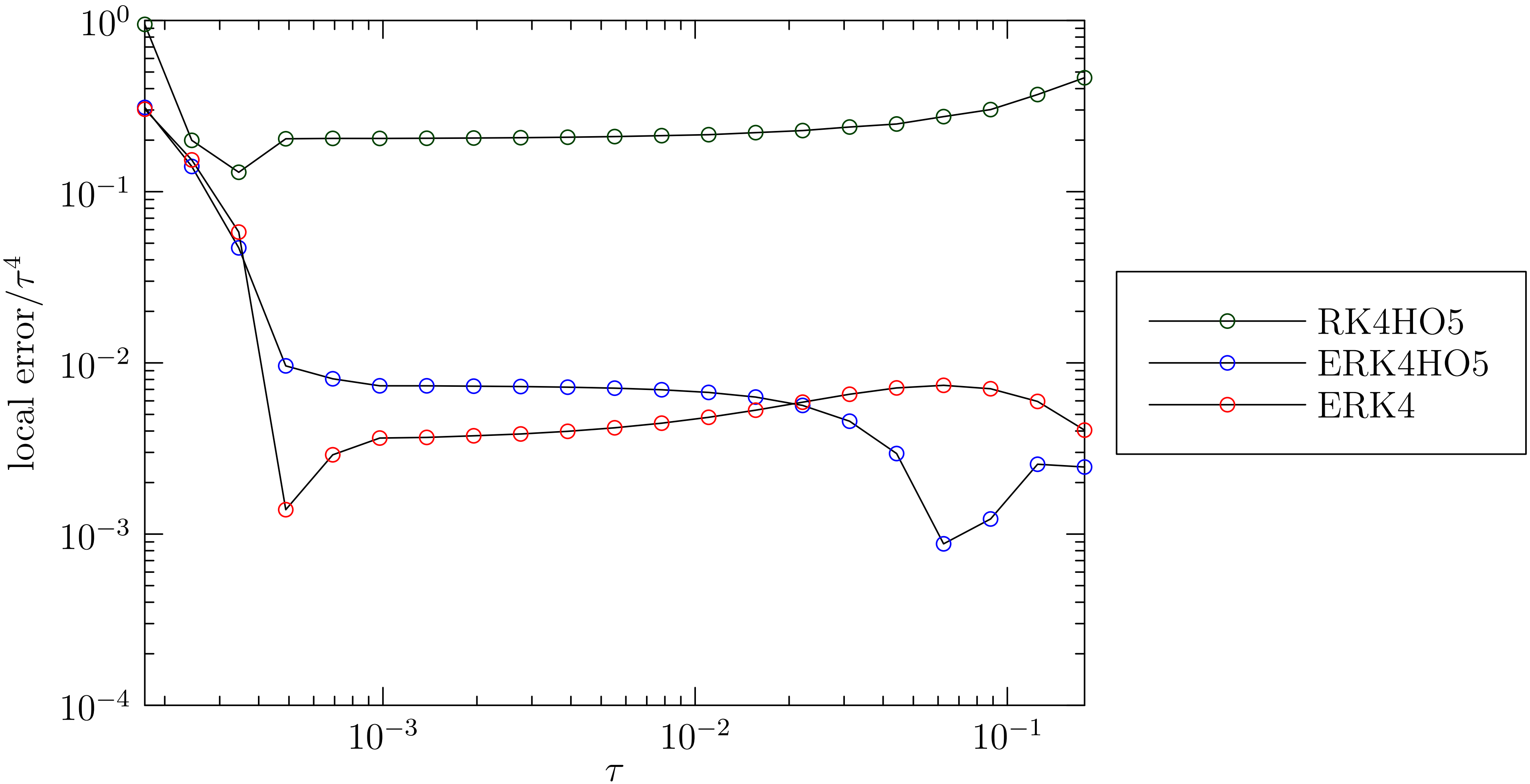
ERK4 integrator with 4 stages

- Let $x = -L\tau$.

$$
\begin{aligned}
a_{00} &= \frac{1}{2}\varphi_1\left(\frac{1}{2}x\right), \\
a_{10} &= \frac{1}{2}\varphi_1\left(\frac{1}{2}x\right) - \varphi_2\left(\frac{1}{2}x\right), \quad && a_{11} = \varphi_2\left(\frac{1}{2}x\right), \\
a_{20} &= \varphi_1(x) - 2\varphi_2(x), && a_{21} = 0, && a_{22} = 2\varphi_2(x), \\
a_{30} &= \varphi_1(x) - 3\varphi_2(x) + 4\varphi_3(x), && a_{31} = a_{32} = 2\varphi_2(x) - 4\varphi_3(x), \\
a_{33} &= -\varphi_2(x) + 4\varphi_3(x),
\end{aligned}
$$

Fourth-order integration test:

$$\frac{dy}{dt} + 6y = -y^2 \qquad y(0) = 1, \qquad t = 1$$



Conclusions

- Exponential integrators are explicit schemes for ODEs with a stiff linearity.
- A general method is proposed for deriving exponential integrators for stiff ordinary differential equations.
- In the scalar case, this technique can be used to develop exponential versions of classical RK integrators, including embedded methods.
- 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.
- A generalization to the vector case is in progress. . . .

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