Exponential Integrators

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May 22, 2007

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Exponential Integrators

- Typical stiff nonlinear initial value problem:

$$\frac{dx}{dt} + \eta\, x = f(t, x), \qquad x(0) = x_0.$$

- Stiff: Nonlinearity f varies slowly in t compared with the value of the linear coefficient η:

$$\left|\frac{1}{f}\frac{df}{dt}\right| \ll |\eta|$$

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

- In the presence of nonlinearity, straightforward integrating factor methods (cf. Lawson 1967) do not remove the explicit restriction on the linear time step τ.

- Instead, discretize the perturbed problem with a scheme that is exact on the time scale of the solvable part.

Exponential Euler Algorithm

- Express exact evolution of x in terms of $P(t) = e^{\eta t}$:

$$x(t) = P^{-1}(t) \left(x_0 + \int_0^t f \, P \, d\bar{t} \right) .$$

- Change variables: $P \, d\bar{t} = \eta^{-1} dP \Rightarrow$

$$x(t) = P^{-1}(t) \left(x_0 + \eta^{-1} \int_1^{P(t)} f \, dP \right) .$$

- Rectangular approximation of integral $\Rightarrow$ Exponential Euler:

$$x_{i+1} = P^{-1} \left(x_i + \frac{P-1}{\eta} f_i \right) ,$$

where $P = e^{\eta \tau}$ and τ is the time step.

- The discretization is now with respect to P instead of t.

Exponential Euler Algorithm (E-Euler)

$$x_{i+1} = P^{-1}x_i + \frac{1 - P^{-1}}{\eta} f(x_i),$$

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

$$x_{i+1} = x_i + \tau f(x_i).$$

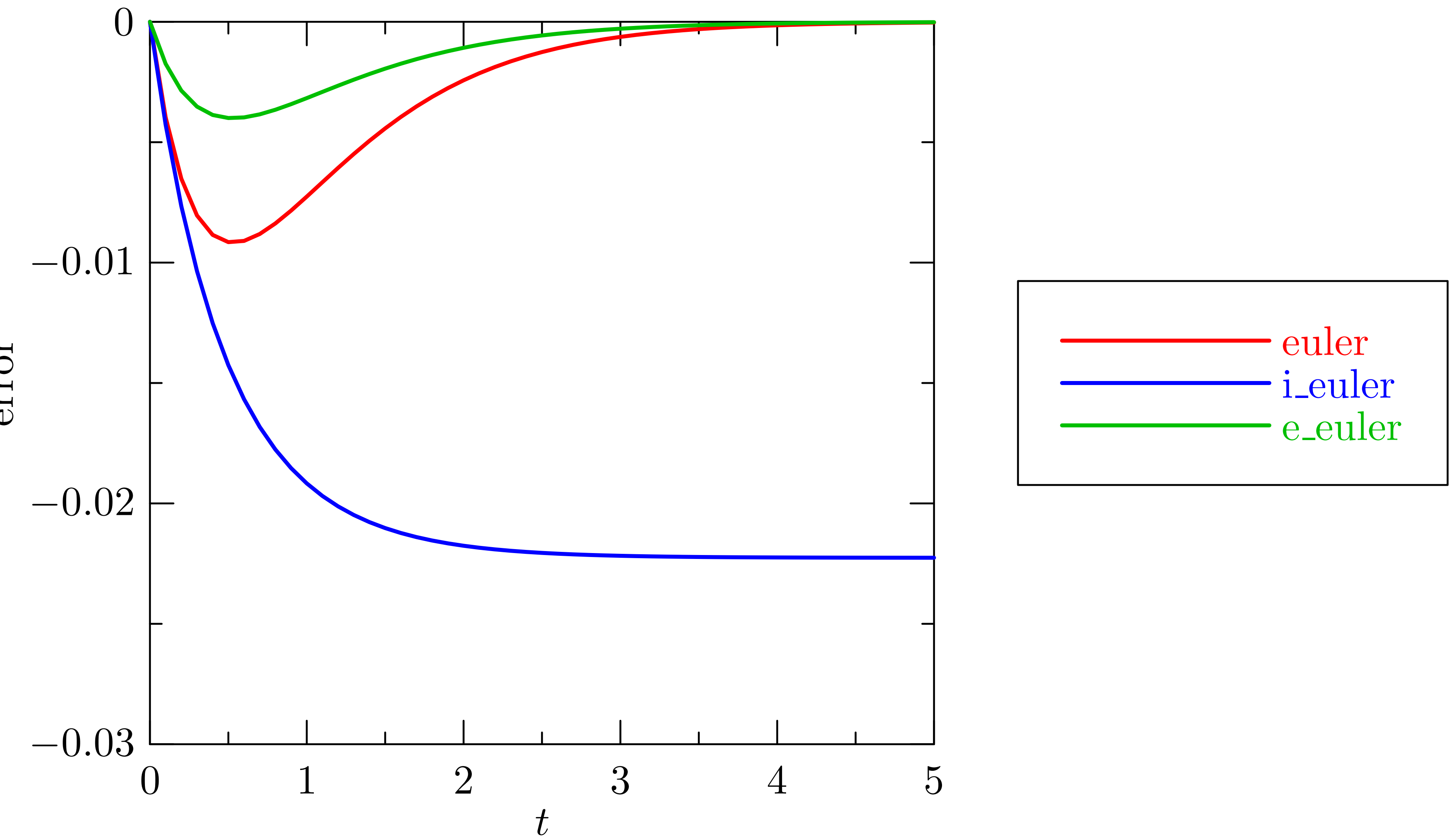
- If E-Euler has a fixed point, it must satisfy $x = \frac{f(x)}{\eta}$; this is then a fixed point of the ODE.
- In contrast, the popular Integrating Factor method (I-Euler).

$$x_{i+1} = P_i^{-1}(x_i + \tau f_i)$$

can at best have an incorrect fixed point: $x = \dfrac{\tau f(x)}{e^{\eta\tau} - 1}$.

Comparison of Euler Integrators

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



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, 2005b]: Explicit Exponential Runge-Kutta; stiff order conditions.

Generalization

- Let $\mathcal{L}$ be a linear operator with a stationary Green's function $G(t,t') = G(t-t')$:

$$\frac{\partial G(t,t')}{\partial t} + \mathcal{L} G(t,t') = \delta(t-t').$$

- Let f be a continuous function of x. Then the ODE

$$\frac{dx}{dt} + \mathcal{L}\, x = f(x), \qquad x(0) = x_0,$$

has the formal solution

$$x(t) = e^{-\int_0^t \mathcal{L}\, dt'} x_0 + \int_0^t G(t-t') f(x(t'))\, dt'.$$

- Letting $s = t - t'$:

$$x(t) = e^{-\int_0^t \mathcal{L}\, dt'} x_0 + \int_0^t G(s) f(x(t-s))\, ds.$$

- Change integration variable to $h = H(s) = \int_0^s G(\bar{s})\, d\bar{s}$:

$$x(t) = e^{-\int_0^t \mathcal{L}\, dt'} x_0 + \int_1^{H(t)} f\big(x(t - H^{-1}(h))\big)\, dh.$$

- Rectangular rule $\Rightarrow$ Predictor (Euler):

$$\widetilde{x}(t) \approx e^{-\int_0^t \mathcal{L}\, dt'} x_0 + f(x(0)) H(t).$$

- Trapezoidal rule $\Rightarrow$ Corrector:

$$x(t) \approx e^{-\int_0^t \mathcal{L}\, dt'} x_0 + \frac{f(x(0)) + f(\widetilde{x}(t))}{2} H(t).$$

Other Generalizations

- Higher-order exponential integrators: Hochbruck *et al.* [1998], Cox & Matthews [2002], Hochbruck & Ostermann [2005a], Bowman *et al.* [2006].
- Vector case (matrix exponential $\boldsymbol{P} = e^{\eta t}$).
- Exponential versions of Conservative Integrators [Bowman *et al.* 1997, Shadwick *et al.* 1999, Kotovych & Bowman 2002].
- Lagrangian discretizations of advection equations are also exponential integrators:

$$\frac{\partial u}{\partial t} + v\frac{\partial}{\partial x}u = f(x,t,u), \qquad u(x,0) = u_0(x).$$

- η now represents the linear operator $v\frac{\partial}{\partial x}$ and

$$\mathcal{P}^{-1}u = e^{-tv\frac{\partial}{\partial x}}u$$

corresponds to the Taylor series of $u(x - vt)$.

Higher-Order Integrators

- General s-stage Runge–Kutta scheme:

$$x_i = x_0 + \tau \sum_{j=0}^{i-1} a_{ij} f(x_j, t + b_j \tau), \quad (i = 1, \ldots, s).$$

- Butcher Tableau (s=4):

$$\begin{array}{c|cccc} b_0 & a_{10} & & & \\ b_1 & a_{20} & a_{21} & & \\ b_2 & a_{30} & a_{31} & a_{32} & \\ b_3 & a_{40} & a_{41} & a_{42} & a_{43} \end{array}$$

Bogacki–Shampine (3,2) Pair

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

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

- Since $f(x_3)$ is just f at the initial x_0 for the next time step, no additional source evaluation is required to compute x_4 [FSAL].

- Also: 6-stage (5,4) pair [Bogacki & Shampine 1996].

Vector Case

- When $\boldsymbol{x}$ is a vector, $\boldsymbol{\nu}$ is typically a matrix:

$$\frac{d\boldsymbol{x}}{dt} + \boldsymbol{\nu}\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}).$$

- Let $\boldsymbol{z} = -\boldsymbol{\nu}\tau$. Discretization involves

$$\varphi_1(\boldsymbol{z}) = \boldsymbol{z}^{-1}(e^{\boldsymbol{z}} - \mathbf{1}).$$

- Higher-order exponential integrators require

$$\varphi_j(\boldsymbol{z}) = \boldsymbol{z}^{-j}\left(e^{\boldsymbol{z}} - \sum_{k=0}^{j-1}\frac{\boldsymbol{z}^k}{k!}\right).$$

- Exercise care when $\boldsymbol{z}$ has an eigenvalue near zero!

- Although a variable time step requires re-evaluation of the matrix exponential, this is not an issue for problems where the evaluation of the nonlinear term dominates the computation.

- Pseudospectral turbulence codes: diagonal matrix exponential.

Charged Particle in Electromagnetic Fields

- Lorentz force:

$$\frac{m}{q}\frac{d\boldsymbol{v}}{dt} = \frac{1}{c}\boldsymbol{v}\times\boldsymbol{B} + \boldsymbol{E}.$$

- Efficiently compute the matrix exponential $\exp(\boldsymbol{\Omega})$, where

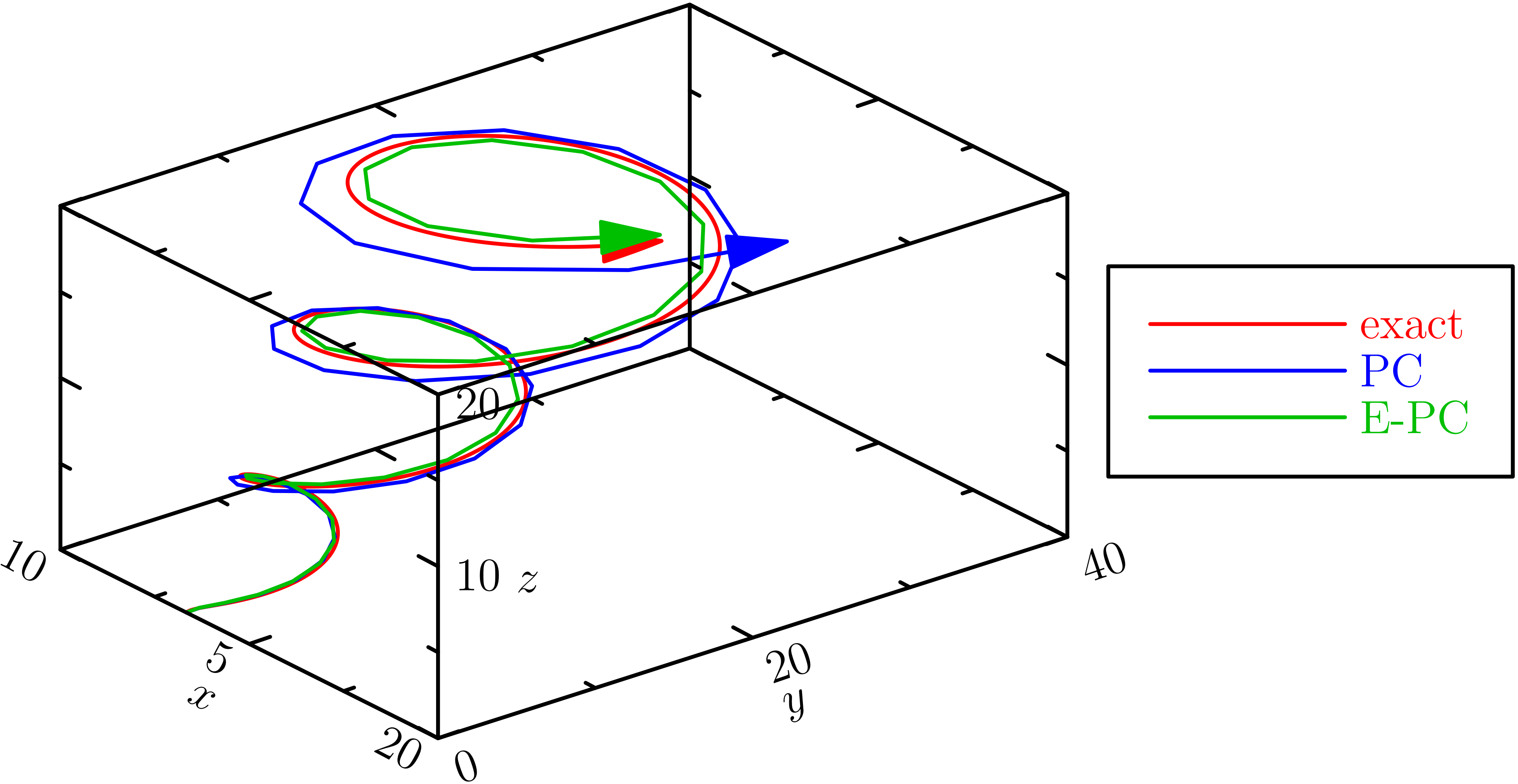
$$\boldsymbol{\Omega} = -\frac{q}{mc}\tau\begin{pmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{pmatrix}.$$

- Requires 2 trigonometric functions, 1 division, 1 square root, and 35 additions or multiplications.

- The other necessary matrix factor, $\boldsymbol{\Omega}^{-1}[\exp(\boldsymbol{\Omega}) - \mathbf{1}]$ requires care, since $\boldsymbol{\Omega}$ is singular. Evaluate it as

$$\lim_{\lambda\to 0}[(\boldsymbol{\Omega} + \lambda\mathbf{1})^{-1}(e^{\boldsymbol{\Omega}} - \mathbf{1})].$$

Motion Under Lorentz Force



An Embedded 4-Stage (3,2) Exponential Pair

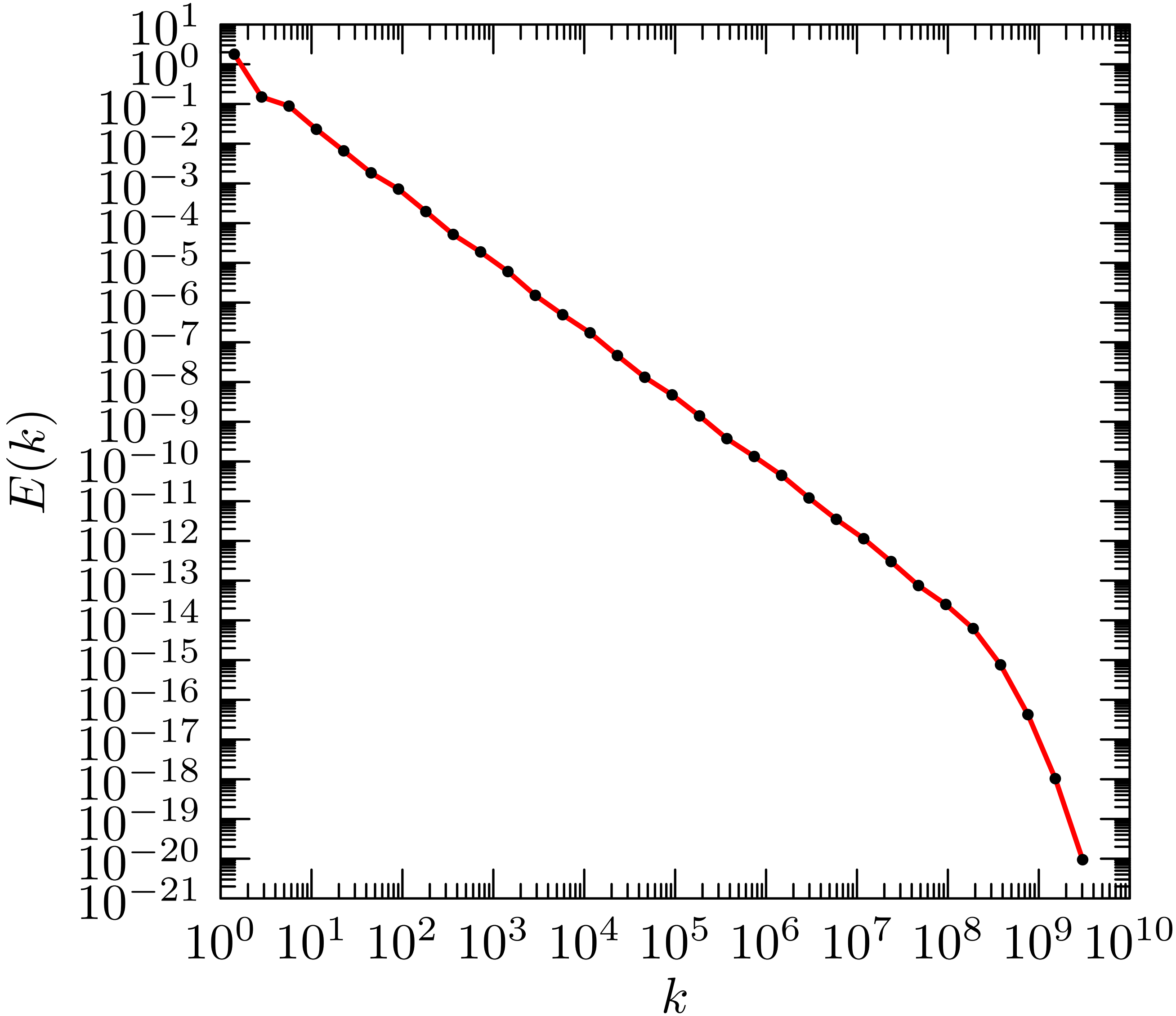
- Letting $\boldsymbol{z} = -\boldsymbol{\nu}\tau$ and $b_4 = 1$:

$$\boldsymbol{x}_i = e^{-b_i\boldsymbol{\nu}\tau}\boldsymbol{x}_0 + \tau\sum_{j=0}^{i-1}\boldsymbol{a}_{ij}f(\boldsymbol{x}_j, t + b_j\tau), \quad (i = 1, \ldots, s).$$

$$\boldsymbol{a}_{10}=\frac{1}{2}\varphi_1\left(\frac{1}{2}\boldsymbol{z}\right),$$
$$\boldsymbol{a}_{20}=\frac{3}{4}\varphi_1\left(\frac{3}{4}\boldsymbol{z}\right) - a_{21},\ \ \boldsymbol{a}_{21}=\frac{9}{8}\varphi_2\left(\frac{3}{4}\boldsymbol{z}\right) + \frac{3}{8}\varphi_2\left(\frac{1}{2}\boldsymbol{z}\right),$$
$$\boldsymbol{a}_{30}=\varphi_1(\boldsymbol{z}) - \boldsymbol{a}_{31} - \boldsymbol{a}_{32},\ \ \boldsymbol{a}_{31}=\frac{1}{3}\varphi_1(\boldsymbol{z}), \boldsymbol{a}_{32}=\frac{4}{3}\varphi_2(\boldsymbol{z}) - \frac{2}{9}\varphi_1(\boldsymbol{z}),$$
$$\boldsymbol{a}_{40}=\varphi_1(\boldsymbol{z}) - \frac{17}{12}\varphi_2(\boldsymbol{z}),\ \ \boldsymbol{a}_{41}=\frac{1}{2}\varphi_2(\boldsymbol{z}),\ \ \boldsymbol{a}_{42}=\frac{2}{3}\varphi_2(\boldsymbol{z}),\ \ \boldsymbol{a}_{43}=\frac{1}{4}\varphi_2(\boldsymbol{z}). \tag{1}$$

- $\boldsymbol{x}_3$ has stiff order 3 [Hochbruck and Ostermann 2005] (order is preserved even when $\boldsymbol{\nu}$ is a general unbounded linear operator).
- $\boldsymbol{x}_4$ provides a second-order estimate for adjusting the time step.
- $\boldsymbol{\nu} \to 0$: reduces to [3,2] Bogacki–Shampine Runge–Kutta pair.

Application to GOY Turbulence Shell Model



Conclusions

- 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 present an efficient adaptive embedded 4-stage (3,2) exponential pair.
- A similar embedded 6-stage (5,4) exponential pair also exists.
- Care must be exercised when evaluating $\varphi_j(x)$ near 0. Accurate optimized double precision routines for evaluating these functions are available at `www.math.ualberta.ca/~bowman/phi.h`

Asymptote: The Vector Graphics Language

`http://asymptote.sf.net`

(freely available under the GNU public license)

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