Structure-Preserving and Exponential Discretizations of Initial-Value Problems

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Outline

Initial Value Problems

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

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, t), \tag{1}$$

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

- If $n = 2k$ 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 $H(\boldsymbol{q}, \boldsymbol{p}, t) : \mathbb{R}^{n+1} \to \mathbb{R}$, we say that (1) is Hamiltonian.

- 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]
- Exponential integrators: Operator splitting yields exact evolution on linear time scale.

Symplectic vs. Conservative Integration

Theorem 1 (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.
- 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:

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

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 $\boldsymbol{x}_0 \in \mathbb{R}^n$ $\exists$ a C^1 function $\phi : \mathbb{R} \to \mathbb{R} \ni$

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

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

$Q.E.D.$

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

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

$$\frac{dx_1}{dt} = f_1 = M_1 x_2 x_3,$$
$$\frac{dx_2}{dt} = f_2 = M_2 x_3 x_1,$$
$$\frac{dx_3}{dt} = f_3 = M_3 x_1 x_2,$$

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

- Energy is not conserved by conventional discretizations.
- The Euler method,

$$x_k(t+\tau) = x_k(t) + \tau f_k,$$

yields a monotonically increasing new energy:

$$E(t+\tau) = \frac{1}{2}\sum_k \left[x_k^2 + 2\tau f_k x_k + \tau^2 S_k^2\right]$$

$$= E(t) + \frac{1}{2}\tau^2 \sum_k S_k^2.$$

Conservative Euler Algorithm

- Determine a modification of the original equations of motion leading to *exact* energy conservation:

$$\frac{dx_k}{dt} = f_k + g_k.$$

- Euler's method predicts the new energy

$$E(t+\tau) = \frac{1}{2}\sum_k \left[x_k + \tau(f_k + g_k)\right]^2$$

$$= E(t) + \frac{1}{2}\sum_k \underbrace{\left[2\tau g_k x_k + \tau^2 (f_k + g_k)^2\right]}_{\text{set to } 0}.$$

- Solving for g_k yields the C–Euler discretization:

$$x_k(t+\tau) = \operatorname{sgn} x_k(t+\tau)\,\sqrt{x_k^2 + 2\tau f_k x_k}.$$

- Reduces to Euler's method as $\tau \to 0$:

$$\begin{aligned} x_k(t+\tau) &= x_k\sqrt{1 + 2\tau\frac{f_k}{x_k}} \\ &= x_k + \tau f_k + \mathcal{O}(\tau^2). \end{aligned}$$

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

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

Lemma 1: *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 m*-stage discretization*

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

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

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 $\boldsymbol{\xi} = \boldsymbol{T}(\boldsymbol{x})$.
- The new value of $\boldsymbol{x}$ is then obtained by inverse transformation:

$$\boldsymbol{x}(t+\tau) = \boldsymbol{T}^{-1}(\boldsymbol{\xi}(t+\tau)).$$

- Problem: T may not be invertible!
  Solution 1: Reduce the time step.
  Solution 2: Switch to 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 x_0):

$$x(t+\tau) = x_0 + \tau f + \frac{\tau^2}{2} f' f + \frac{\tau^3}{6}(f'' f^2 + f'^2 f) + \mathcal{O}(\tau^4);$$

- When $T'(x_0) \neq 0$, C–PC yields the solution

$$x(t+\tau) = x_0 + \tau f + \frac{\tau^2}{2} f' f + \frac{\tau^3}{4}\left(f'' f^2 + \frac{T'''}{3T'} f^3\right) + \mathcal{O}(\tau^4),$$

  where all of the derivatives are evaluated at x_0.

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

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

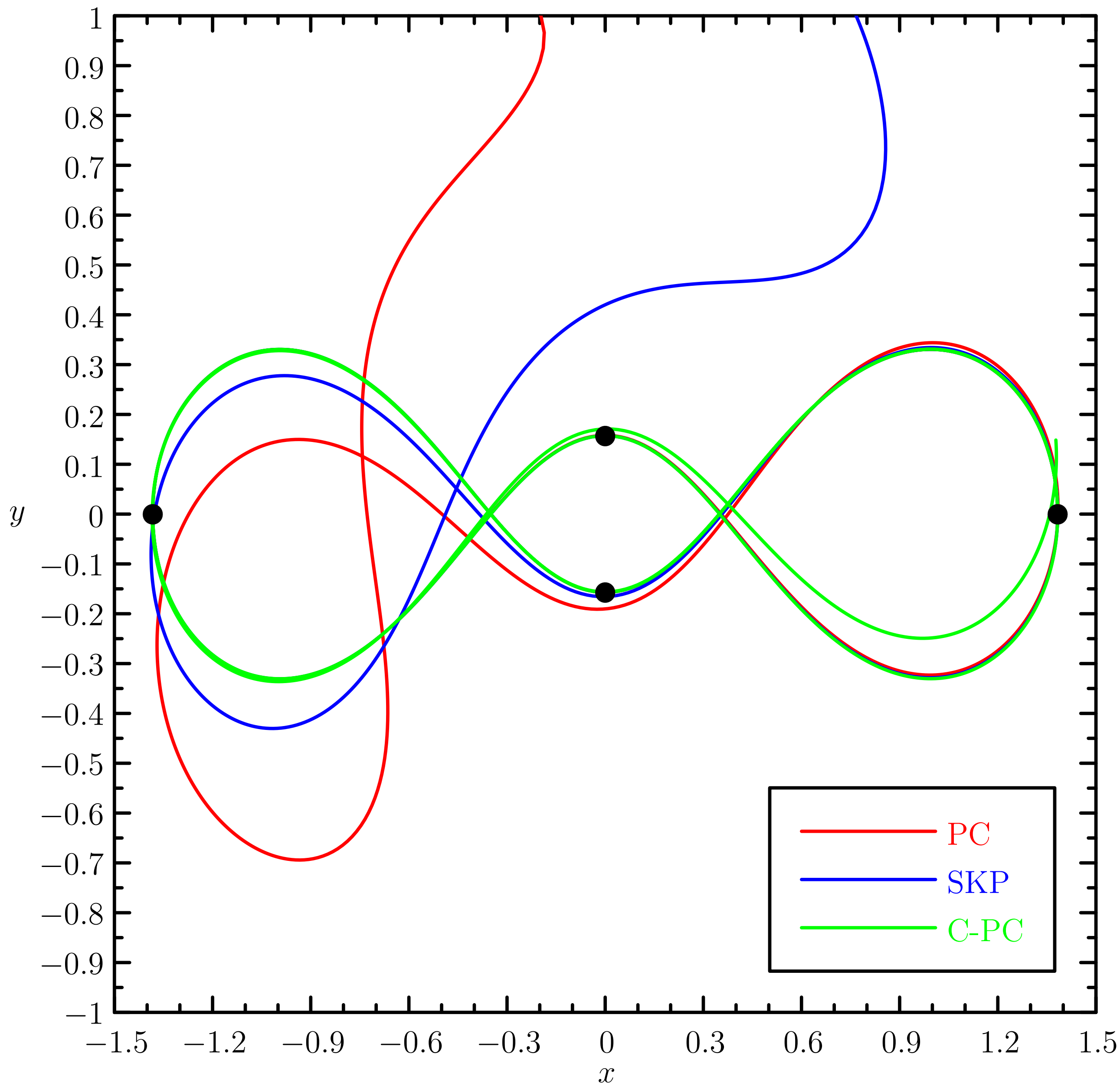
Singular Case

- When $T'(x_0) = 0$, the conservative corrector reduces to

$$x(t+\tau) = T^{-1}\left(T(x_0) + \frac{\tau}{2}T'(\tilde{x})f(\tilde{x})\right),$$

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

Four-Body Choreography



PC, symplectic SKP, and C–PC solutions

Conservative Symplectic Integrators

- Conservative variational symplectic integrators based on explicitly time-dependent symplectic maps have been proposed for certain mechanics problems. [Kane, Marsden, and Ortiz 1999]
- These integrators circumvent the conditions of the Ge–Marsden theorem!

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 do not remove the explicit restriction on the linear time step τ.

Exponential Euler Algorithm

- Exact evolution of x:

$$x(t_0+\tau) = P^{-1}(t_0+\tau)\left[x(t_0) + \int_{t_0}^{t_0+\tau} dt\, P(t) f(t)\right],$$

where $P(t) = e^{\eta(t-t_0)}$.

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

$$x(t_0+\tau) = P^{-1}(t_0+\tau)\left[x(t_0) + \eta^{-1}\int_{1}^{P(t_0+\tau)} dP\, f\right].$$

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

$$x_{i+1} = P_{i+1}^{-1}\left[x_i + \eta^{-1}(P_{i+1}-1) f_i\right].$$

- The discretization is now with respect to P instead of t.
- Also known as the Exponentially Fitted Euler method.

Generalizations

- Higher-order exponential integrators: [Hochbruck and Lubich 1997, Cox and Matthews 2004, Hochbruck and Ostermann 2005, Bowman 2005].
- Vector case (matrix exponential $\boldsymbol{P} = e^{\boldsymbol{\eta} t}$).
- Gaussian Quadrature with respect to weight function P.
- Conservative Exponential Integrators
- Can replace linear Green's function $e^{\eta(t-t')}$ by any *stationary* Green's function $G(t-t')$.
- 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 $u(x-vt)$.

Charged Particle in Electromagnetic Fields

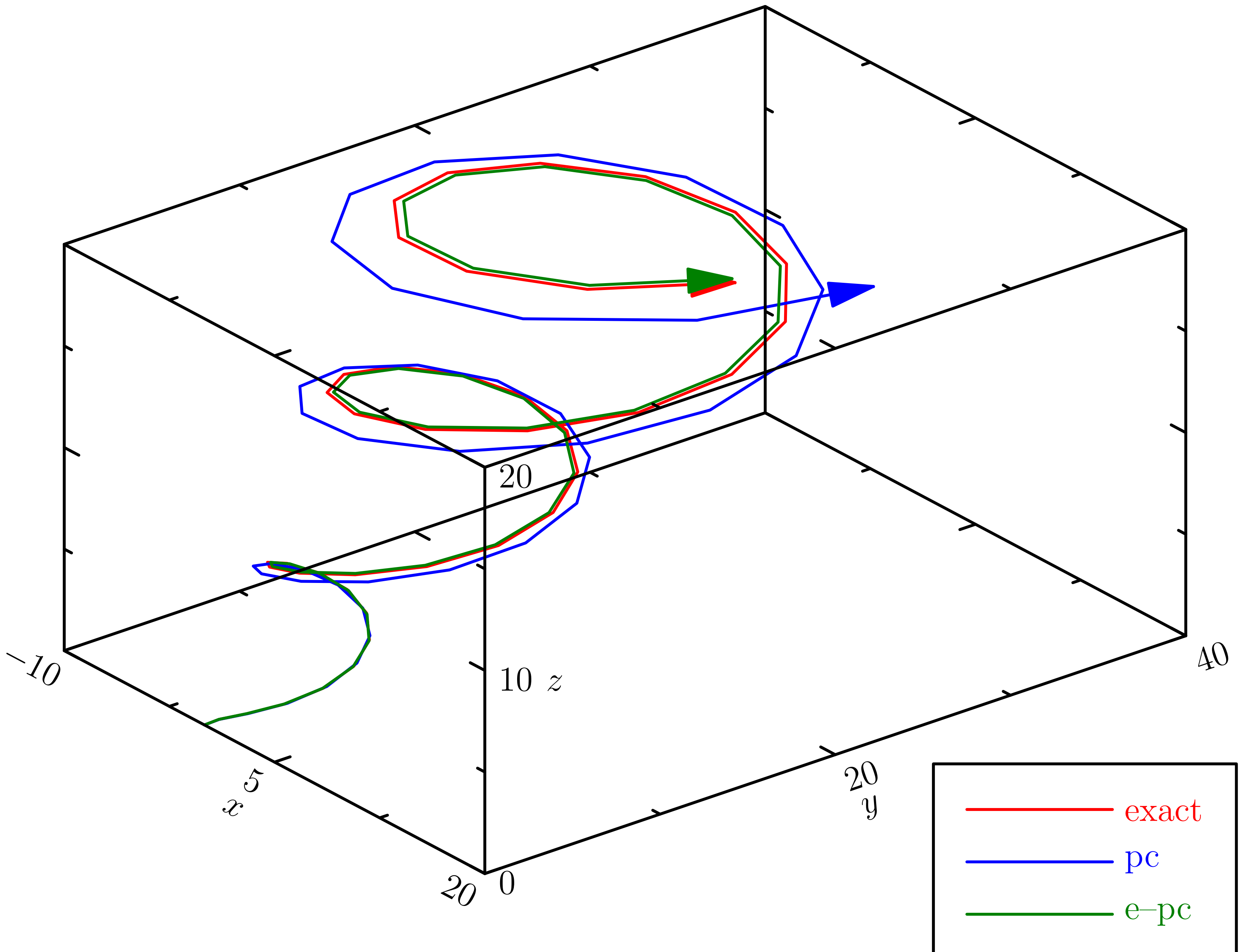
- Lorentz force:
$$\frac{m}{q}\frac{d\boldsymbol{v}}{dt} = \frac{1}{c}\boldsymbol{v}\times\boldsymbol{B} + \boldsymbol{E}.$$

- Efficiently compute the matrix exponential $\exp(\boldsymbol{\Omega})$, where
$$\boldsymbol{\Omega} = -\frac{q}{mc}t\begin{pmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{pmatrix}.$$

- 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



Higher-Order Exponential Integrators

- Vector case:

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

- Autonomous Runge–Kutta scheme:

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

- Matrix functions

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

and

$$\varphi_2(\boldsymbol{x}) = \boldsymbol{x}^{-2}(e^{\boldsymbol{x}} - \mathbf{1} - \boldsymbol{x}).$$

- Exercise care when evaluating φ_1 and φ_2 near zero!

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

$$\boldsymbol{a}_{10} = \frac{1}{2}\varphi_1\left(\frac{1}{2}\boldsymbol{x}\right),$$

$$\boldsymbol{a}_{20} = \frac{3}{4}\varphi_1\left(\frac{3}{4}\boldsymbol{x}\right) - a_{21},\ \boldsymbol{a}_{21} = \frac{9}{8}\varphi_2\left(\frac{3}{4}\boldsymbol{x}\right) + \frac{3}{8}\varphi_2\left(\frac{1}{2}\boldsymbol{x}\right),$$

$$\boldsymbol{a}_{30} = \varphi_1(\boldsymbol{x}) - \boldsymbol{a}_{31} - \boldsymbol{a}_{32},\ \boldsymbol{a}_{31} = \frac{1}{3}\varphi_1(\boldsymbol{x}), \boldsymbol{a}_{32} = \frac{4}{3}\varphi_2(\boldsymbol{x}) - \frac{2}{9}\varphi_1(\boldsymbol{x}),$$

$$\boldsymbol{a}_{40} = \varphi_1(\boldsymbol{x}) - \frac{17}{12}\varphi_2(\boldsymbol{x}),\ \boldsymbol{a}_{41} = \frac{1}{2}\varphi_2(\boldsymbol{x}),\ \boldsymbol{a}_{42} = \frac{2}{3}\varphi_2(\boldsymbol{x}),\ \boldsymbol{a}_{43} = \frac{1}{4}\varphi_2(\boldsymbol{x}),$$

- $\boldsymbol{x}_3$ has stiff order 3 [Hochbruck and Ostermann 2005].
- $\boldsymbol{x}_4$ provides a second-order estimate for adjusting the time step.
- Since $\boldsymbol{f}(\boldsymbol{x}_3)$ is just $\boldsymbol{f}$ at the initial $\boldsymbol{x}_0$ for the next time step, no additional source evaluation is required to compute $\boldsymbol{x}_4$ [FSAL].
- $\boldsymbol{\eta} \to 0$: reduces to [3,2] Bogacki–Shampine Runge–Kutta pair.

Asymptote: The Vector Graphics Language

`http://asymptote.sf.net`

(freely available under the GNU public license)

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