Structure-Preserving Discretizations of Initial-Value Problems

John C. Bowman (University of Alberta)

March 29, 2012

www.math.ualberta.ca/∼bowman/talks

Outline

- Structure-Preserving Discretizations
- Symplectic Integrators
- Conservative Integrators
- Exponential Integrators
  - Exponential Euler
  - History
- Generalizations
  - Stationary Green Function
  - Higher-Order
  - Vector Case
  - Lagrangian Discretizations
- Charged Particle in Electromagnetic Fields

- Embedded Exponential Runge–Kutta (3,2) Pair
- 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 $\boldsymbol{x}(0) = \boldsymbol{x}_0$.

- 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 Eq. () 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]

- Positivity: preserves positive semi-definiteness of covariance matrices. [Bowman & Krommes 1997]

- Unitary integration: conserves trace of probability density matrix. [Shadwick & Buell 1997]

- 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

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

where

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

- 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:

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

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

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

- 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: 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 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.

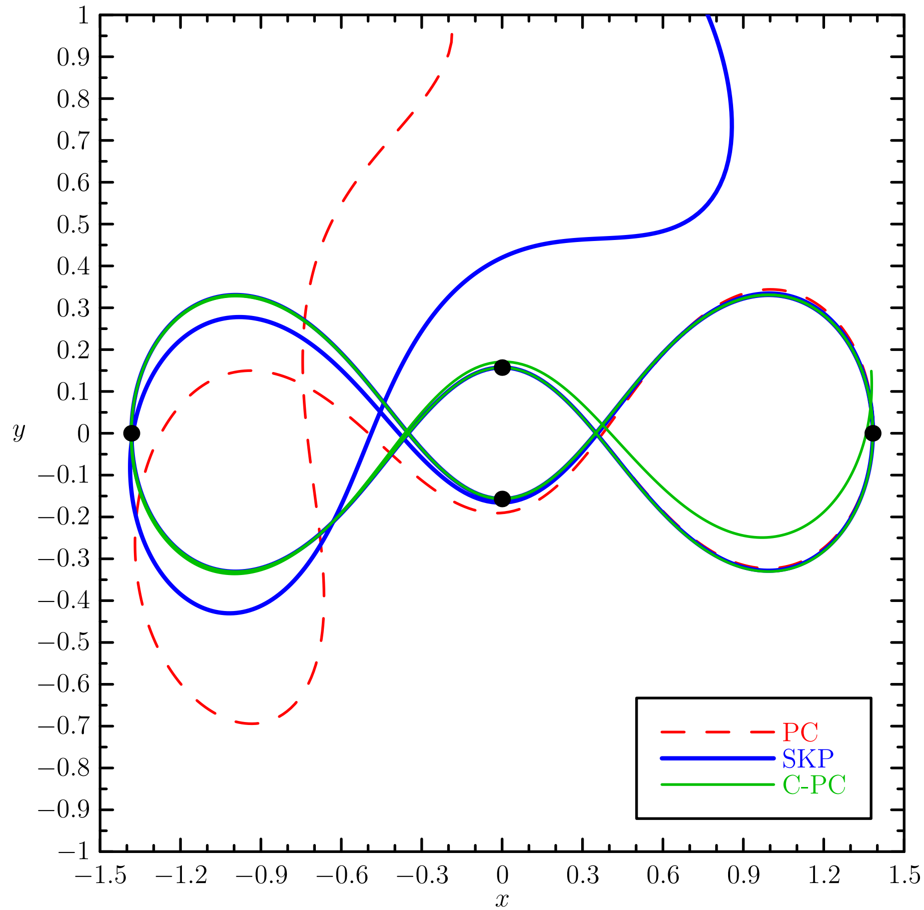
Singular Case

- 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:

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

- 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 y in terms of $P(t) = e^{\eta t}$:

$$y(t) = P^{-1}(t)\left(y_0 + \int_0^t f\,P\,d\bar{t}\right).$$

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

$$y(t) = P^{-1}(t)\left(y_0 + \eta^{-1}\int_1^{P(t)} f\,dP\right).$$

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

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

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)

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

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

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

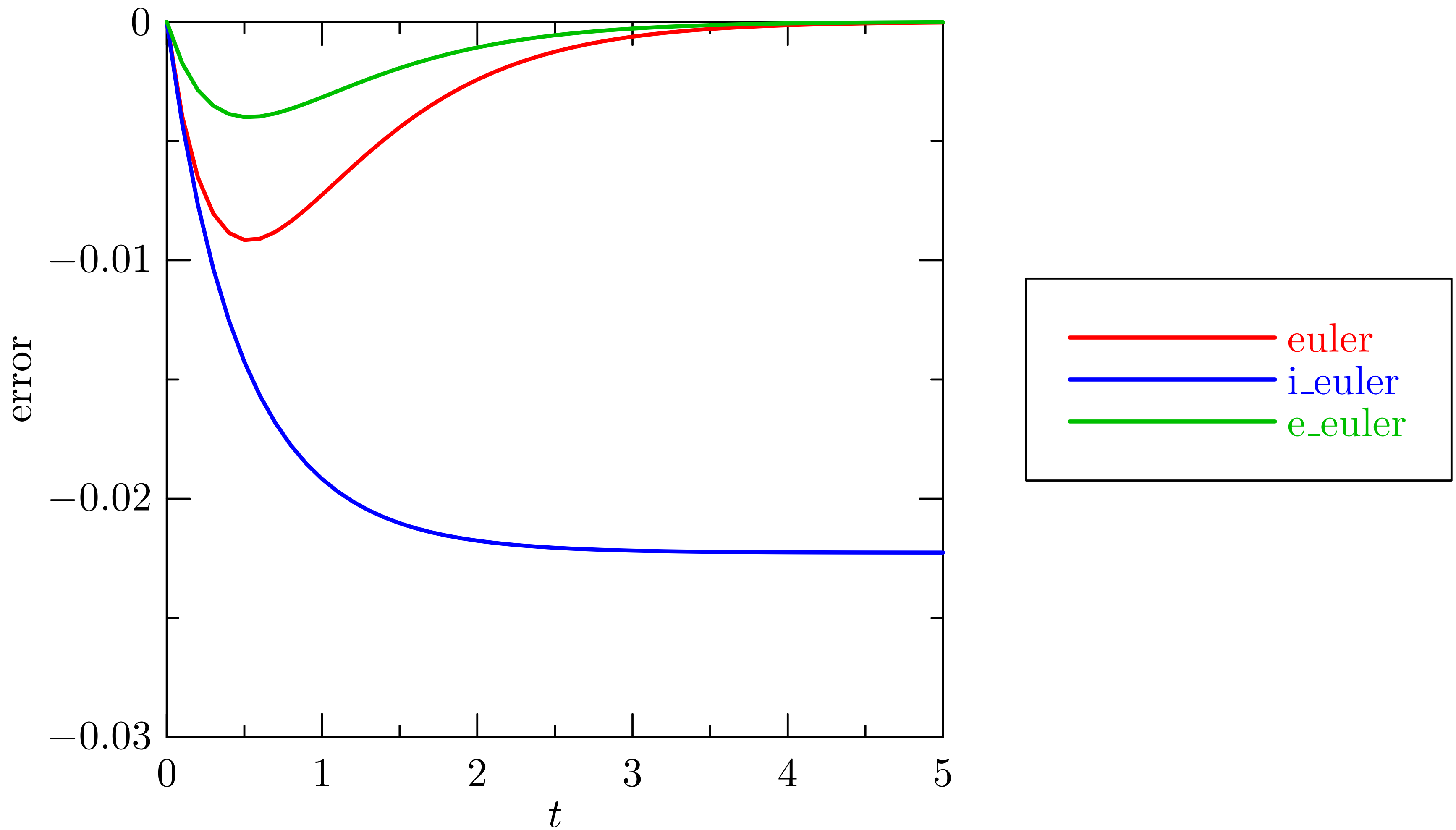
- If E-Euler has a fixed point, it must satisfy $y = \frac{f(y)}{\eta}$; this is then a fixed point of the ODE.
- In contrast, the popular Integrating Factor method (I-Euler).

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

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

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], Hochbruck & Ostermann [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 y. Then the ODE

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

has the formal solution

$$y(t) = e^{-\int_0^t \mathcal{L}\,dt'} y_0 + \int_0^t G(t-t') f(y(t'))\,dt'.$$

- Letting $s = t - t'$:

$$y(t) = e^{-\int_0^t \mathcal{L}\, dt'} y_0 + \int_0^t G(s) f(y(t-s))\, ds.$$

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

$$y(t) = e^{-\int_0^t \mathcal{L}\, dt'} y_0 + \int_1^{H(t)} f\big(y(t - H^{-1}(h))\big)\, dh.$$

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

$$\widetilde{y}(t) \approx e^{-\int_0^t \mathcal{L}\, dt'} y_0 + f(y(0)) H(t).$$

- Trapezoidal rule $\Rightarrow$ Corrector:

$$y(t) \approx e^{-\int_0^t \mathcal{L}\, dt'} y_0 + \frac{f(y(0)) + f(\widetilde{y}(t))}{2} H(t).$$

Other Generalizations

- Higher-order exponential integrators: Hochbruck *et al.* [1998], Cox & Matthews [2002], Hochbruck & Ostermann [2005a], Bowman *et al.* [2006].

- Vector case (matrix exponential $\boldsymbol{P} = e^{\boldsymbol{\eta} t}$).

- 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 $v\frac{\partial}{\partial x}$

$\mathcal{P}^{-1}u = e^{-tv\frac{\partial}{\partial x}}u$ corresponds to the Taylor series of $u(x - vt)$.

Higher-Order Integrators

- General s-stage Runge–Kutta scheme:

$$y_i = y_0 + \tau \sum_{j=0}^{i-1} a_{ij} f(y_j, t + b_j \tau), \quad (i = 1, \ldots, s).$$

- Butcher Tableau (s=4):

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

Higher-Order Exponential Integrators

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

- Let $x = e^{\eta t}$, $u = xy$. Then $dx/dt = \eta x$, so that

$$\frac{du}{dx} = \frac{d(xy)}{dx} = y + x\frac{dt}{dx}\frac{dy}{dt} = y + \frac{1}{\eta}(f - \eta y) = \frac{f}{\eta}$$

- Apply conventional integrator to

$$\frac{du}{dx} = \frac{f}{\eta}.$$

- When y is evolved from $t = 0$ to $t = \tau$, the new independent variable goes from $x = 1$ to $x = e^{\eta\tau}$.

Vector Case

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

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

- 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

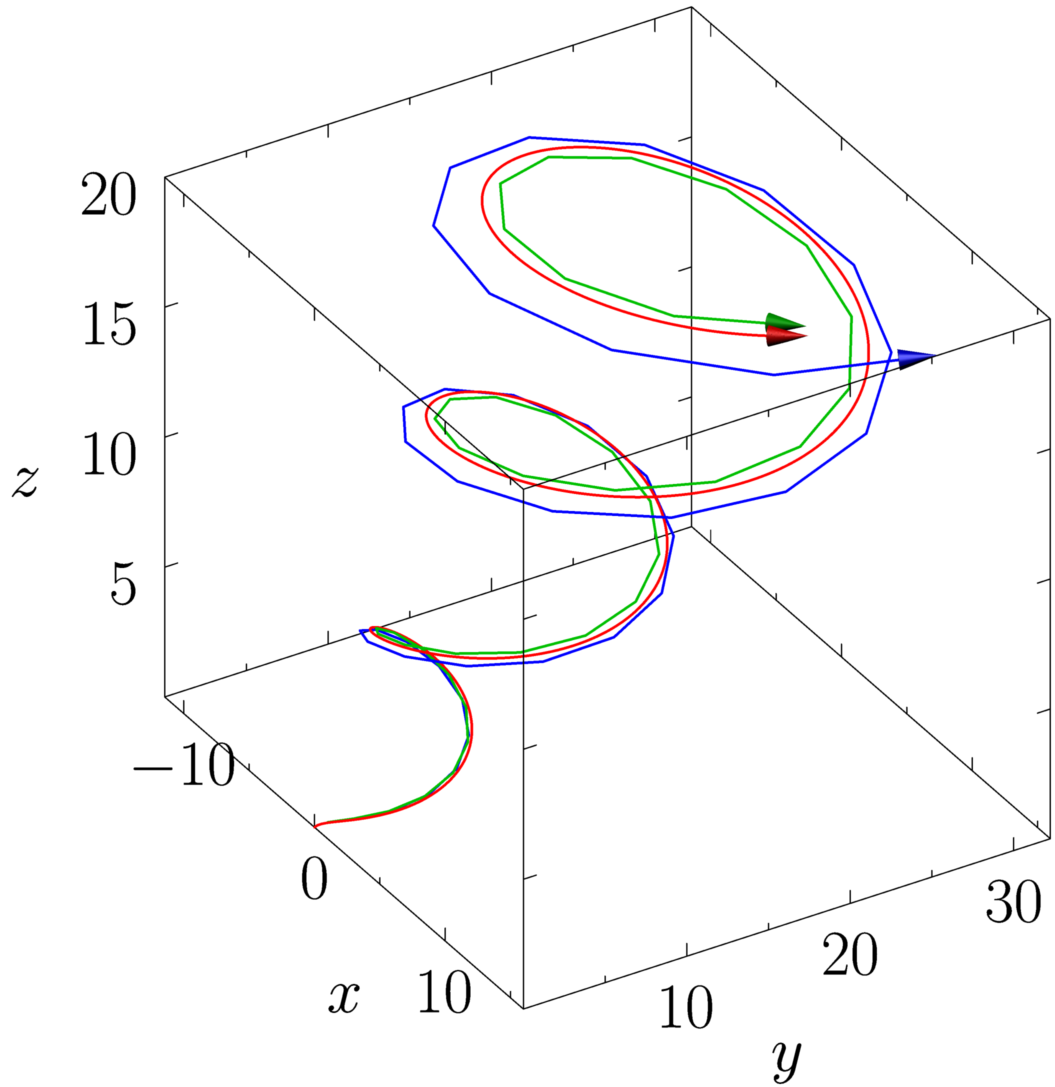
$$\boldsymbol{\Omega} = -\frac{q}{mc}\tau\begin{pmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{pmatrix}.$$

- 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



Exact, PC, E-PC trajectories of a particle under Lorentz force.

Bogacki–Shampine (3,2) Pair

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

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

- Since $f(y_3)$ is just f at the initial y_0 for the next time step, no additional source evaluation is required to compute y_4 [FSAL].

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

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

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

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

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

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

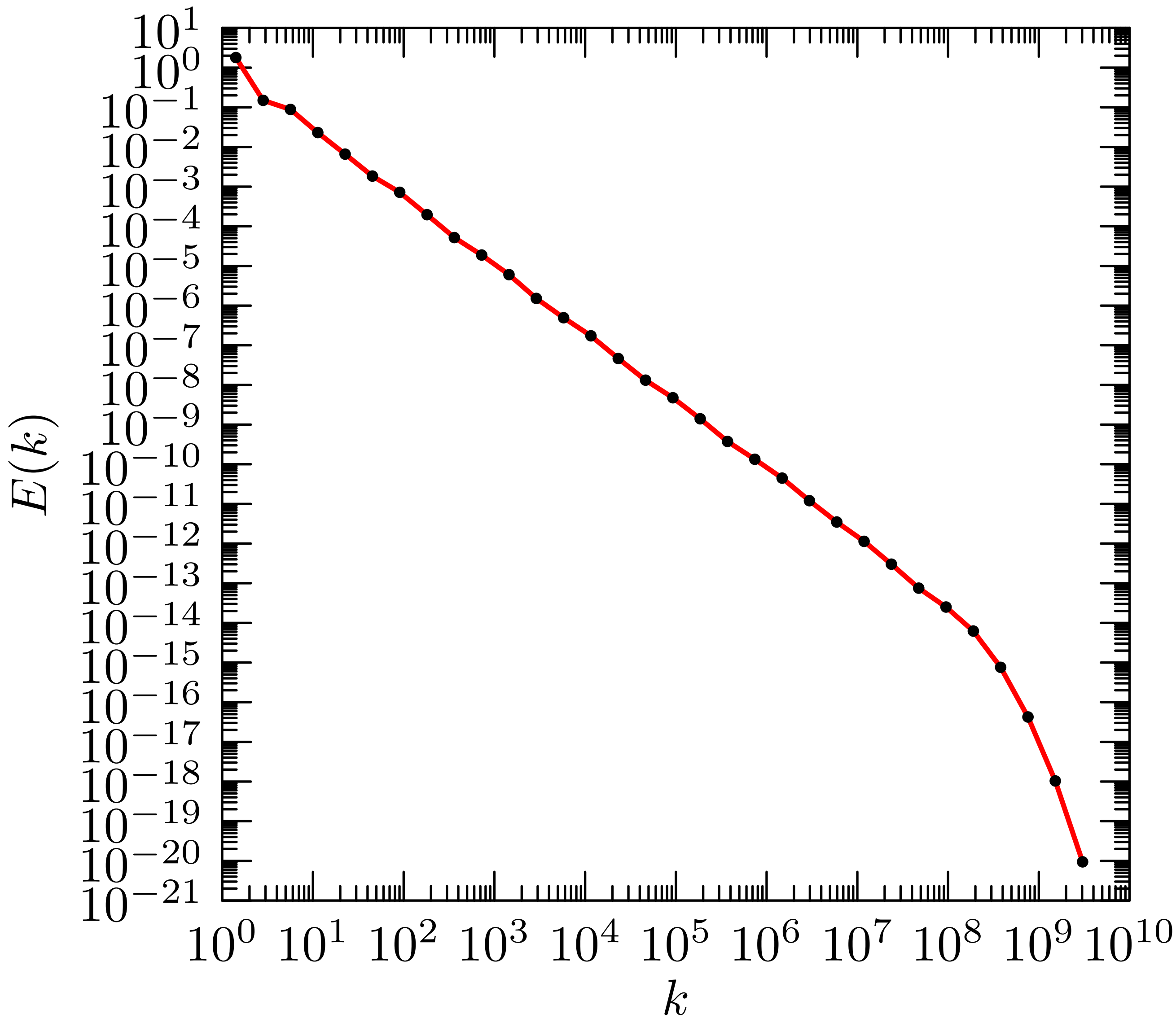
$$\boldsymbol{a}_{40} = \varphi_1(\boldsymbol{z}) - \frac{17}{12}\varphi_2(\boldsymbol{z}), \;\; \boldsymbol{a}_{41} = \frac{1}{2}\varphi_2(\boldsymbol{z}), \;\; \boldsymbol{a}_{42} = \frac{2}{3}\varphi_2(\boldsymbol{z}), \;\; \boldsymbol{a}_{43} = \frac{1}{4}\varphi_2(\boldsymbol{z}).$$

- $\boldsymbol{y}_3$ has stiff order 3 [Hochbruck and Ostermann 2005] (order is preserved even when $\boldsymbol{\nu}$ is a general unbounded linear operator).

- $\boldsymbol{y}_4$ provides a second-order estimate for adjusting the time step.

- $\boldsymbol{\nu} \to \mathbf{0}$: reduces to [3,2] Bogacki–Shampine Runge–Kutta pair.

Application to GOY Turbulence Shell Model



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 present an efficient adaptive embedded 4-stage (3,2) exponential pair.
- Work is under way to develop an embedded 6-stage (5,4) exponential pair.
- Care must be exercised when evaluating φ_j near 0. Accurate optimized double precision routines for evaluating these functions are available at `www.math.ualberta.ca/~bowman/phi.h`

Asymptote: 2D & 3D Vector Graphics Language

Andy Hammerlindl, John C. Bowman, Tom Prince

`http://asymptote.sf.net`

(freely available under the GNU public license)

Asymptote Lifts TeX to 3D

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2}\,dx = \sqrt{\frac{\pi}{\alpha}}$$

Acknowledgements: Orest Shardt (U. Alberta)

References

[Beylkin *et al.* 1998] G. Beylkin, J. M. Keiser, & L. Vozovoi, J. Comp. Phys., **147**:362, 1998.

[Bogacki & Shampine 1989] P. Bogacki & L. F. Shampine, Appl. Math. Letters, **2**:1, 1989.

[Bowman & Krommes 1997] J. C. Bowman & J. A. Krommes, Phys. Plasmas, **4**:3895, 1997.

[Bowman *et al.* 1993] J. C. Bowman, J. A. Krommes, & M. Ottaviani, Phys. Fluids B, **5**:3558, 1993.

[Bowman *et al.* 1997] J. C. Bowman, B. A. Shadwick, & P. J. Morrison, "Exactly conservative integrators," in *15th IMACS World Congress on Scientific Computation, Modelling and Applied Mathematics*, edited by A. Sydow, volume 2, pp. 595–600, Berlin, 1997, Wissenschaft & Technik.

[Bowman *et al.* 2006] J. C. Bowman, C. R. Doering, B. Eckhardt, J. Davoudi, M. Roberts, & J. Schumacher, Physica D, **218**:1, 2006.

[Certaine 1960] J. Certaine, Math. Meth. Dig. Comp., p. 129, 1960.

[Channell & Scovel 1990] P. J. Channell & J. C. Scovel, Nonlinearity, **3**:231, 1990.

[Cox & Matthews 2002] S. Cox & P. Matthews, J. Comp. Phys., **176**:430, 2002.

[Friedli 1978] A. Friedli, Lecture Notes in Mathematics, **631**:214, 1978.

[Ge Zhong & Marsden 1988] Ge Zhong & J. E. Marsden, Phys. Lett. A, **133**:134, 1988.

[Hochbruck & Ostermann 2005a] M. Hochbruck & A. Ostermann, SIAM J. Numer. Anal., **43**:1069, 2005.

[Hochbruck & Ostermann 2005b] M. Hochbruck & A. Ostermann, Appl. Numer. Math., **53**:323, 2005.

[Hochbruck *et al.* 1998] M. Hochbruck, C. Lubich, & H. Selfhofer, SIAM J. Sci. Comput., **19**:1552, 1998.

[Kane *et al.* 1999] C. Kane, J. E. Marsden, & M. Ortiz, J. Math. Phys., **40**:3353, 1999.

[Kotovych & Bowman 2002] O. Kotovych & J. C. Bowman, J. Phys. A.: Math. Gen., **35**:7849, 2002.

[Lu 2003] Y. Y. Lu, J. Comput. Appl. Math., **161**:203, 2003.

[Nørsett 1969] S. Nørsett, Lecture Notes in Mathematics, **109**:214, 1969.

[Ruth 1983] R. D. Ruth, IEEE Trans. Nucl. Sci., **NS-30**:2669, 1983.

[Sanz-Serna & Calvo 1994] J. M. Sanz-Serna & M. P. Calvo, *Numerical Hamiltonian Problems*, volume 7 of *Applied Mathematics and Mathematical Computation*, Chapman and Hall, London, 1994.

[Shadwick & Buell 1997] B. A. Shadwick & W. F. Buell, Phys. Rev. Lett., **79**:5189, 1997.

[Shadwick *et al.* 1999] B. A. Shadwick, J. C. Bowman, & P. J. Morrison, SIAM J. Appl. Math., **59**:1112, 1999.

[van der Houwen 1977] P. J. van der Houwen, *Construction of integration formulas for initial value problems*, North-Holland Publishing Co., Amsterdam, 1977, North-Holland Series in Applied Mathematics and Mechanics, Vol. 19.

[Verwer 1977] J. Verwer, Numer. Math., **27**:143, 1977.