Structure-Preserving and Exponential Discretizations of Initial-Value Problems

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Outline

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Initial Value Problems

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

\[
\frac{d}{dt} x = f(x, t),
\]

with the initial condition \( x(0) = x_0 \).

- If \( n = 2k \) and \( x = (q, p) \) where \( q, p \in \mathbb{R}^k \) satisfy

\[
\begin{align*}
\frac{dq}{dt} &= \frac{\partial H}{\partial p}, \\
\frac{dp}{dt} &= -\frac{\partial H}{\partial q},
\end{align*}
\]

for some function \( H(q, p, t) : \mathbb{R}^{n+1} \to \mathbb{R} \), 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]


- **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 $\tilde{H}_\tau(x, t) : \mathbb{R}^{n+1} \to \mathbb{R}$, where the label $\tau$ denotes the time step.
- If the mapping $M$ does not depend explicitly on time, it can be generated by the approximate Hamiltonian $K(x) = \tilde{H}_\tau(x, 0)$.  


Suppose the symplectic map conserves the true Hamiltonian $H$:

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

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 $x_0 \in \mathbb{R}^n$

$\exists$ a $C^1$ function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ $\exists$

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

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).

⇒ 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:

\[
\frac{dx_1}{dt} = f_1 = M_1x_2x_3, \\
\frac{dx_2}{dt} = f_2 = M_2x_3x_1, \\
\frac{dx_3}{dt} = f_3 = M_3x_1x_2,
\]

where \( M_1 + M_2 + M_3 = 0 \).

- Then

\[
\sum_k f_k x_k = 0 \Rightarrow \text{energy } E = \frac{1}{2} \sum_k x_k^2 \text{ is conserved.}
\]
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
  \[ E(t + \tau) = \frac{1}{2} \sum_k [x_k + \tau (f_k + g_k)]^2 \]
  \[ = E(t) + \frac{1}{2} \sum_k \left[ 2\tau g_k x_k + \tau^2 (f_k + g_k)^2 \right]. \]
  Set to 0
Solving for \( g_k \) yields the C–Euler discretization:

\[
x_k(t + \tau) = \text{sgn} \ x_k(t + \tau) \sqrt{x_k^2 + 2\tau f_k x_k}.
\]

Reduces to Euler’s method as \( \tau \to 0 \):

\[
x_k(t + \tau) = x_k \sqrt{1 + 2\tau \frac{f_k}{x_k}}
= x_k + \tau f_k + O(\tau^2).
\]

C–Euler is just the usual Euler algorithm applied to

\[
\frac{dx_k^2}{dt} = 2f_k x_k.
\]
Lemma 1: Let $\mathbf{x}$ and $\mathbf{c}$ be vectors in $\mathbb{R}^n$. If $\mathbf{f} : \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ has values orthogonal to $\mathbf{c}$, so that $I = \mathbf{c} \cdot \mathbf{x}$ is a linear invariant of
\[
\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t),
\]
then each stage of the explicit $m$-stage discretization
\[
\mathbf{x}_i = \mathbf{x}_0 + \tau \sum_{j=0}^{i-1} a_{ij} \mathbf{f}(\mathbf{x}_j, t + a_i \tau), \quad i = 1, \ldots, m,
\]
also conserves $I$, where $\tau$ is the time step and $a_{ij} \in \mathbb{R}$. 
Higher-Order Conservative Integration

- Find a transformation $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that the nonlinear invariants are linear functions of $\xi = T(x)$.
- The new value of $x$ is then obtained by inverse transformation:
  \[ x(t + \tau) = T^{-1}(\xi(t + \tau)). \]

Problem: $T$ may not be invertible!
Solution 1: Reduce the time step.
Solution 2: Switch to a traditional integrator for that time step.

- 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 $x_0$):

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

- 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 $\tau$; for $T(x) = x^2$, they agree through third order in $\tau$. 

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:
  \[ \frac{dx}{dt} + \eta x = f(t, x), \quad x(0) = x_0. \]
  
- **Stiff**: Nonlinearity \( f \) varies slowly in \( t \) compared with the value of the linear coefficient \( \eta \):
  \[ \left| \frac{1}{f} \frac{df}{dt} \right| \ll |\eta|. \]
  
- **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 \( \tau \).
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: $dt \ P = \eta^{-1} dP$ ⇒

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

Rectangular approximation of integral ⇒ 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

- **Vector case** (matrix exponential $P = e^{\eta t}$).
- Gaussian Quadrature with respect to weight function $P$.
- Conservative Exponential Integrators
- Can replace linear Green’s function $e^{\eta(t-t')} \eta$ by any stationary Green’s function $G(t - t')$.
- Lagrangian discretizations of advection equations are also exponential integrators:
  \[
  \frac{\partial u}{\partial t} + v \frac{\partial}{\partial x} u = f(x, t, u), \quad u(x, 0) = u_0(x).
  \]
- $\eta$ now represents the linear operator $v \frac{\partial}{\partial x}$ and $P^{-1} u = e^{-t v \frac{\partial}{\partial x}} u$ corresponds to the Taylor series of $u(x - vt)$. 
Charged Particle in Electromagnetic Fields

- Lorentz force:
  \[
  \frac{m}{q} \frac{dv}{dt} = \frac{1}{c} \mathbf{v} \times \mathbf{B} + \mathbf{E}.
  \]

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

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

- The other necessary matrix factor, \( \Omega^{-1}[\exp(\Omega) - 1] \) requires care, since \( \Omega \) is singular. Evaluate it as
  \[
  \lim_{\lambda \to 0} [(\Omega + \lambda \mathbf{1})^{-1}(e^{\Omega} - 1)].
  \]
Motion under Lorentz force
Higher-Order Exponential Integrators

- Vector case:
  \[ \frac{dx}{dt} + \eta x = f(x). \]

- Autonomous Runge–Kutta scheme:
  \[ x_i = x_0 + \tau \sum_{j=0}^{i-1} a_{ij} f(x_j), \quad (i = 1, \ldots, s). \]

- Matrix functions
  \[ \varphi_1(x) = x^{-1}(e^x - 1) \]
  \[ \text{and} \]
  \[ \varphi_2(x) = x^{-2}(e^x - 1 - x). \]

- Exercise care when evaluating \( \varphi_1 \) and \( \varphi_2 \) near zero!
An Embedded 4-Stage (3,2) Exponential Pair

\[ a_{10} = \frac{1}{2} \varphi_1 \left( \frac{1}{2} x \right), \]
\[ a_{20} = \frac{3}{4} \varphi_1 \left( \frac{3}{4} x \right) - a_{21}, \quad a_{21} = \frac{9}{8} \varphi_2 \left( \frac{3}{4} x \right) + \frac{3}{8} \varphi_2 \left( \frac{1}{2} x \right), \]
\[ a_{30} = \varphi_1(x) - a_{31} - a_{32}, \quad a_{31} = \frac{1}{3} \varphi_1(x), \quad a_{32} = \frac{4}{3} \varphi_2(x) - \frac{2}{9} \varphi_1(x), \]
\[ a_{40} = \varphi_1(x) - \frac{17}{12} \varphi_2(x), \quad a_{41} = \frac{1}{2} \varphi_2(x), \quad a_{42} = \frac{2}{3} \varphi_2(x), \quad a_{43} = \frac{1}{4} \varphi_2(x), \]

- \( x_3 \) has stiff order 3 [Hochbruck and Ostermann 2005].
- \( x_4 \) provides a second-order estimate for adjusting the time step.
- 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].
- \( \eta \to 0 \): 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)
References


