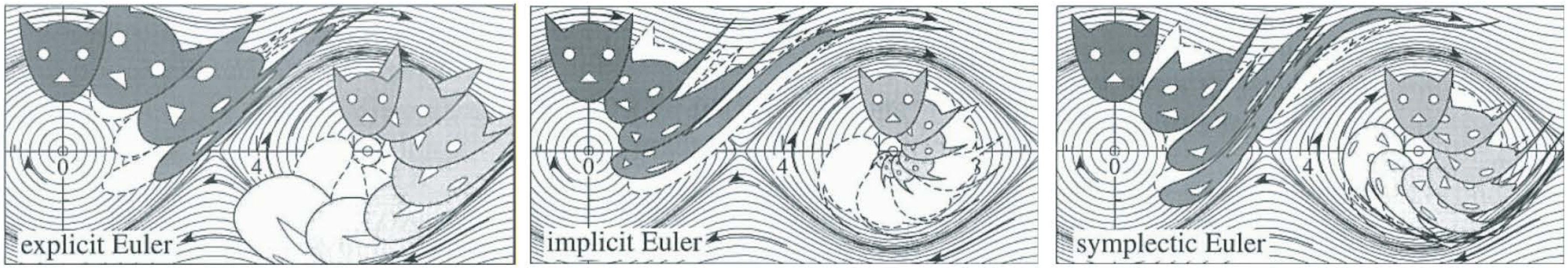


Figure 3: *Symplecticity [reproduced from [Hairer et al. 2002]]: while a continuous Lagrangian system is symplectic (that is to say, in this simple case, an area in phase space evolves along the flow without changing its area), discrete time integrators rarely share this property. From our three time integrators compared in Section 3, only the last one is symplectic. In the background, the reader will recognize the shape of the orbits obtained in Fig. 1(right).*

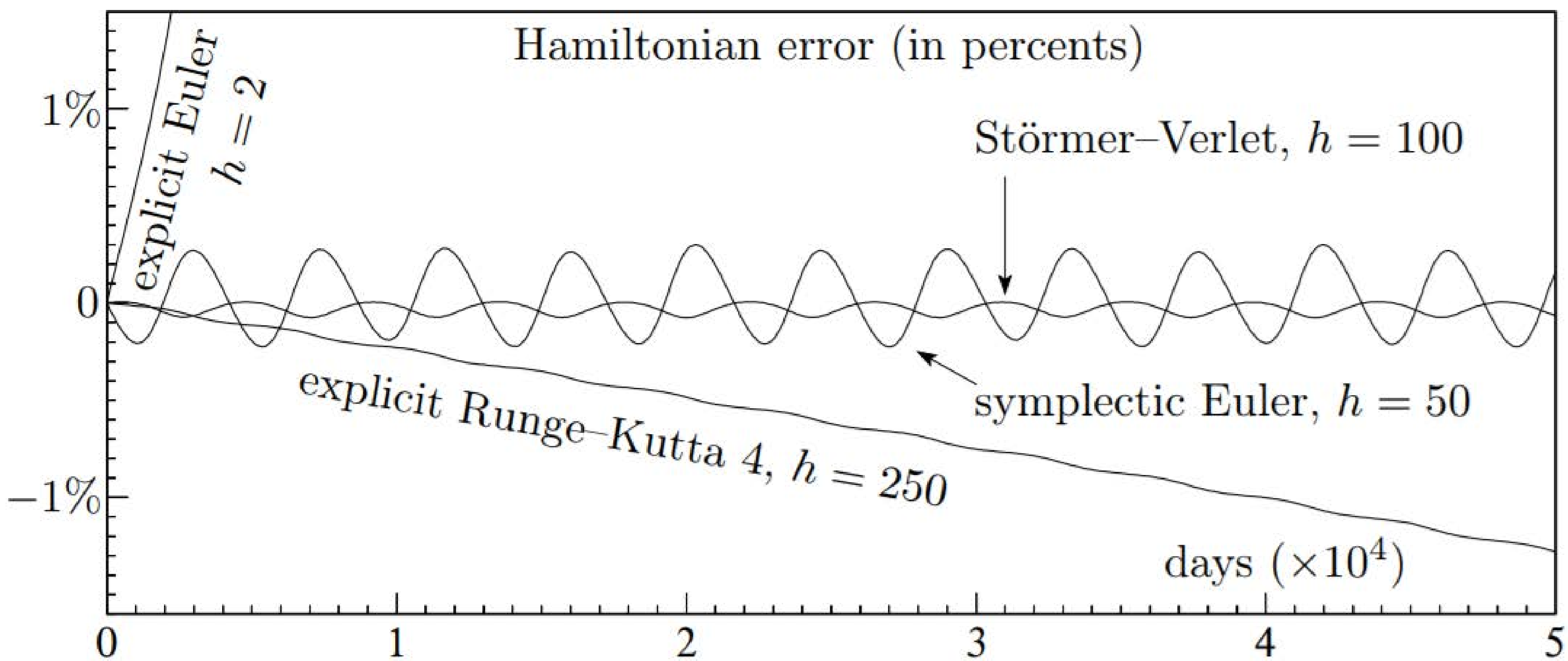


Figure 3: Energy conservation for the three-body problem Sun-Jupiter-Saturn.

Symplectic integrators.

Ex. Symplectic Euler.

① $$\begin{cases} p_{n+1} = p_n - h \nabla_q H(p_{n+1}, q_n) \\ q_{n+1} = q_n + h \nabla_p H(p_{n+1}, q_n) \end{cases}$$

looks like implicit.

If $H(p,q) = T(p) + V(q)$

$$\begin{cases} p_{n+1} = p_n - h \nabla_q V(q_n) \\ q_{n+1} = q_n + h \nabla_p T(p_{n+1}) \end{cases}$$

explicit.

already obtained

symplectic. order 1 (HW)

Hint: $\underline{X} \in \mathbb{R}^{d\times d}$. $\underline{X} = \underline{X}^T$.

$$\begin{pmatrix} I & 0 \\ \underline{X} & I \end{pmatrix}^T J \begin{pmatrix} I & 0 \\ \underline{X} & I \end{pmatrix} = J = \begin{pmatrix} I & \underline{X} \\ 0 & I \end{pmatrix}^T J \begin{pmatrix} I & \underline{X} \\ 0 & I \end{pmatrix}$$

② $$\begin{cases} p_{n+1} = p_n - h \nabla_q H(p_n, q_{n+1}) \overset{\text{when separable}}{=} p_n - h \nabla_q V(q_{n+1}) \\ q_{n+1} = q_n + h \nabla_p H(p_n, q_{n+1}) = q_n + h \nabla_p T(p_n) \end{cases}$$

first evaluate $\longrightarrow$ explicit.

Ex. Strömer-Verlet

$$\begin{cases} p_{n+\frac{1}{2}} = p_n - \frac{h}{2} \nabla_q H(p_{n+\frac{1}{2}}, q_n) \\ q_{n+1} = q_n + \frac{h}{2} \left(\nabla_p H(p_{n+\frac{1}{2}}, q_n) + \nabla_p H(p_{n+\frac{1}{2}}, q_{n+1}) \right) \end{cases}$$

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2} D_q H(p_{n+\frac{1}{2}}, q_{n+1})$$

Similar version which evaluates $q_{n+\frac{1}{2}}$ first.

(exer)

H separable. explicit.

symp. order 2.

why symp? Rewrite Strömer-Verlet

$$\begin{cases} p_{n+\frac{1}{2}} = p_n - \frac{h}{2} D_q H(p_{n+\frac{1}{2}}, q_n) \\ q_{n+\frac{1}{2}} = q_n + \frac{h}{2} D_p H(p_{n+\frac{1}{2}}, q_n) \end{cases} \longrightarrow \begin{pmatrix} p_{n+\frac{1}{2}} \\ q_{n+\frac{1}{2}} \end{pmatrix} = \Psi^{(1)}_{\frac{h}{2}} \begin{pmatrix} p_n \\ q_n \end{pmatrix}$$

$$\begin{cases} p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2} \nabla_q H(p_{n+\frac{1}{2}}, q_{n+1}) \\ q_{n+1} = q_{n+\frac{1}{2}} + \frac{h}{2} \nabla_p H(p_{n+\frac{1}{2}}, q_{n+1}) \end{cases} \longrightarrow \begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = \Psi^{(2)}_{\frac{h}{2}} \begin{pmatrix} p_{n+\frac{1}{2}} \\ q_{n+\frac{1}{2}} \end{pmatrix}$$

$$u_n = \begin{pmatrix} p_n \\ q_n \end{pmatrix}$$

$$u_{n+1} = \Psi^{SV}_h u_n = \left[\Psi^{(2)}_{\frac{h}{2}} \circ \Psi^{(1)}_{\frac{h}{2}} \right] u_n$$

symp.

composition is also symp.

Ex. GL 1.

$$\begin{cases} k_n = f\left(u_n + \frac{1}{2} h k_n\right) = J^{-1} \nabla H\left(u_n + \frac{1}{2} h k_n\right) \\ u_{n+1} = u_n + h k_n \end{cases}$$

$$\Phi_n = \frac{\partial u_n}{\partial u_0}, \qquad \Xi_n = \frac{\partial k_n}{\partial u_0}$$

Need to show

$$\Phi_{n+1}^T J \Phi_{n+1} = \Phi_n^T J \Phi_n$$

$$\begin{cases} \Phi_{n+1} = \Phi_n + h \Xi_n \\ \Xi_n = J^{-1} \underbrace{\nabla^2 H\left(u_n + \frac{1}{2} h k_n\right)} \cdot \left(\Phi_n + \frac{1}{2} h \Xi_n\right) \end{cases}$$

G_n : Hessian . sym . invertible .

$$\Phi_n = G_n^{-1} J \Xi_n - \frac{1}{2} h \Xi_n$$

$$\Phi_{n+1}^T J \Phi_{n+1} = (\Phi_n^T + h \Xi_n^T) J (\Phi_n + h \Xi_n)$$

$$= \Phi_n^T J \Phi_n + h \left(\Xi_n^T (-J) \cancel{G_n^{-1}} - \frac{1}{2} h \Xi_n^T \right) \cancel{J} \Xi_n$$

$$+ h \Xi_n^T J \left(G_n^{-1} \cancel{J} \Xi_n - \cancel{\frac{1}{2} h} \Xi_n \right)$$

$$+ h^2 \Xi_n^T \cancel{J} \Xi_n$$

$$= \Phi_n^T J \Phi_n \qquad \square .$$

Symplectic Runge-Kutta.

<u>Def</u> (First integral, a.k.a. conserved quantity)

$\dot{u} = f(u)$. $I : \mathbb{R}^d \to \mathbb{R}$. is a first integral

if $\nabla I(u) \cdot f(u) = 0$, $\forall u$.

$$\frac{d}{dt} I(u(t)) = \nabla I(u(t)) \cdot \dot{u}(t) = f(u(t)) \cdot \nabla I(u(t)) = 0.$$

$\Rightarrow I(u(t)) = I(u(0))$ is conserved.

Def (Quadratic first integral).

$I(u) = u^T C u$ for some symmetric matrix C, is a first integral.

Thm (Bochev-Scovel) If RK conserves all possible quadratic first integrals. then RK is symplectic.

Pf: Notes online by Hairer.

basic idea: quadratic first integral.

$$\Phi_n^T J \Phi_n = J \quad \text{for any } n.$$

variational eq.

$$\dot{u} = f(u) \qquad \Phi(t) = \frac{\partial u(t)}{\partial u_0}$$

$$\begin{cases} \dot{\Phi}(t) = \nabla f(u(t))\, \Phi(t) \\ \Phi(0) = \Phi_0 . \end{cases}$$

only need to show RK to discretize are the same.

$\square$.

Thm. All G-L RK are symplectic.

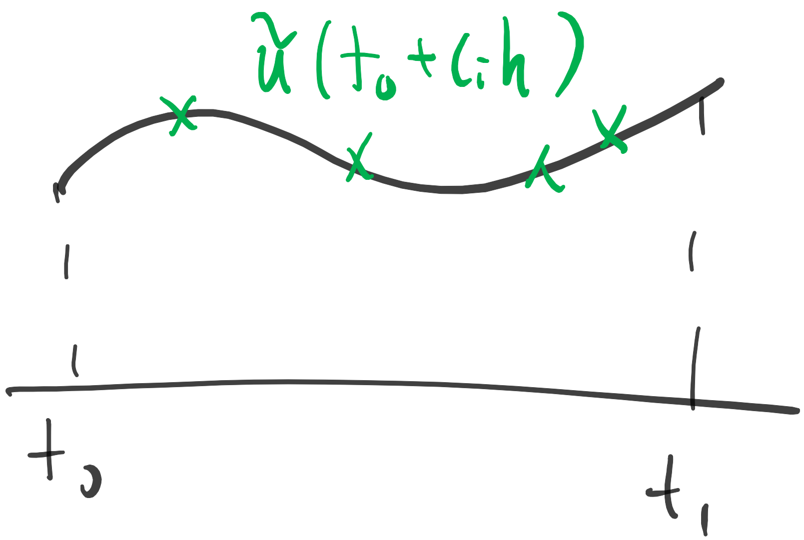
pf: Only need to prove

$I(u) = u^T C u$. is first integral.

then it is preserved by RK.

$$\frac{d}{dt} I(u(t)) = 2u^T C \dot{u} = 2u^T C f = 0.$$

G-L. $\tilde{u}(t)$, $\tilde{u}(t_0) = u_0$, $\tilde{u}(t_1) = u_1$



collocation condition satisfied.

$$\tilde{u}(t_0+c_i h)^T C\, f(\tilde{u}(t_0+c_i h)) = 0, \quad \forall i=1,\dots,r$$

$$u_1^T C u_1 - u_0^T C u_0 = 2\int_{t_0}^{t_1} \underbrace{\tilde{u}(s)^T C\, \dot{\tilde{u}}(s)}_{\text{poly order } 2r-1}\, ds$$

$$= 2\sum_{i=1}^{r} w_i\, \tilde{u}(t_0+c_i h)^T C\, f(\tilde{u}(t_0+c_i h))$$

$$= 0 \qquad \square.$$

Backward error analysis.

$$\dot{u} = f(u) \longrightarrow u(t_n)$$

$$u_{n+1} = \Phi_h(u_n) \longrightarrow u_n$$

① $u(t_{n+1}) - \Phi_h(u(t_n))$. LTE

② Propagate initial error w. LTE to t_n. $\longrightarrow$ $u(t_n) - U_n$

forward error analysis.

Backward error analysis provides a possible way to preserve structure of eq.

$$U_1, U_2, \cdots, U_n, U_{n+1}$$

$\tilde{u}(t)$ continuous. $\tilde{u}(t_n) = U_n$

$$\dot{\tilde{u}}(t) = f_h(\tilde{u}(t))$$

Backward error.

$$f_h(\tilde{u}) = f(\tilde{u}) + \overbrace{h f_2(\tilde{u}) + h^2 f_3(\tilde{u}) + \cdots}$$

series usually diverge.

asymptotic series

formal analysis: treat this as a convergent series.

How to obtain modified eq?

$$\tilde{u} \equiv \tilde{u}(t_n) = u_n, \quad f \equiv f(\tilde{u}(t_n)), \dots$$

Taylor

$$\tilde{u}(t_{n+1}) = \tilde{u} + h\left(f + h f_2 + h^2 f_3 + \cdots\right)$$

method independent

$$+ \frac{h^2}{2}\left(f' + h f_2' + \cdots\right)\left(f + h f_2 + \cdots\right) + \cdots$$

$$\|$$

$$\Phi_h(\tilde{u}) = \tilde{u} + h f + h^2 d_2(\tilde{u}) + h^3 d_3(\tilde{u}) + \cdots$$

method dependent

$$\Rightarrow \begin{cases} f_2 = d_2 - \frac{1}{2} f' f \\ f_3 = d_3 - \frac{1}{3!}\left(f''f^2 + f'^2 f\right) - \frac{1}{2!}\left(f' f_2 + f_2' f\right) \\ \cdots \end{cases}$$

<u>Thm</u>. $u_{n+1} = \Psi_h(u_n)$ order p, then modified eq.

$$f_2 = f_3 = \cdots = f_p \equiv 0, \text{ i.e.}$$

$$\dot{\tilde{u}} = f(\tilde{u}) + h^p f_{p+1}(\tilde{u}) + O(h^{p+1})$$

Pf: Connect w. LTE

$$u(t_{n+1}) - \Psi_h(u_n) \sim O(h^{p+1})$$

$$\Phi_h(u(t_n)) = \tilde{u}(t_n) + \int_{t_n}^{t_{n+1}} f_h(\tilde{u}(s))\,ds. \qquad \tilde{u}(t_n) = u(t_n)$$

$$= \underbrace{\tilde{u}(t_n) + \int_{t_n}^{t_{n+1}} f(\tilde{u}(s))\,ds}_{u(t_{n+1})}$$

$$+ h\int_{t_n}^{t_{n+1}} \cancel{f_2}(\tilde{u}(s))\,ds + \cancel{\cdots} + h^{p-1}\int_{t_n}^{t_{n+1}} \cancel{f_p}(\tilde{u}(s))\,ds$$

$$+ h^{p}\int_{t_n}^{t_{n+1}} f_{p+1}(\tilde{u}(s))\,ds + O(h^{p+2})$$

$\square$

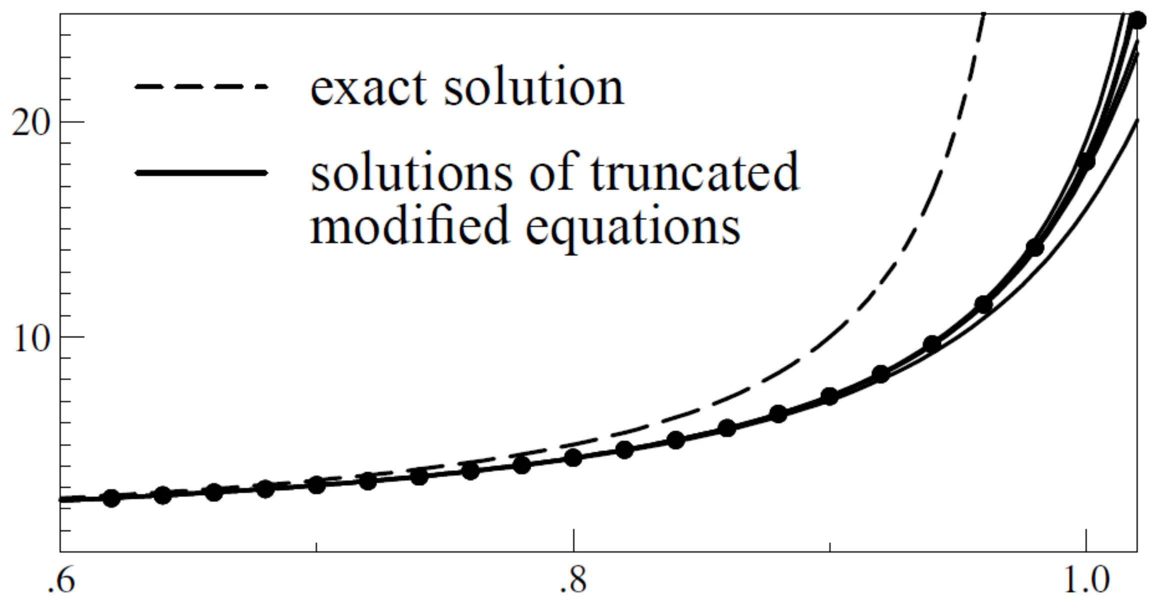


Figure 1: Solutions of the modified equation for the problem $\dot{y} = y^2$, $y(0) = 1$.

Sketch:

symplectic scheme $u_{n+1} = \Phi_h(u_n)$

$$\Downarrow$$

modified eq. $\dot{\tilde{u}} = f_h(\tilde{u})$ $\tilde{u} = (p, q)^T$

$$\Downarrow$$

$$f_h(\tilde{u}) = J^{-1} \nabla \tilde{H}(\tilde{u})$$

modified Hamiltonian.
not far away from H

$$\Downarrow$$

discrete dynamics preserves a modified energy "indefinitely"

$$\Downarrow$$

modified energy stays close to true energy over long time.

Integrability lemma.

For simplicity, consider $\mathbb{R}^n$.

<u>Thm</u>. $f: \mathbb{R}^n \to \mathbb{R}^n$. $f \in C^1(\mathbb{R}^n)$,

$\nabla f(u)$ is symmetric for all $u \in \mathbb{R}^n$. i.e.

$$\frac{\partial f_i}{\partial u_j}(u) = \frac{\partial f_j}{\partial u_i}(u)$$

Then there exists $H: \mathbb{R}^n \to \mathbb{R}$ s.t.

$$f(u) = \nabla H(u)$$

Pf: Define

$$H(u) = \int_0^1 u \cdot f(tu)\, dt + \text{const}$$

$$\frac{\partial H}{\partial u_j} = \int_0^1 f_j(tu) + t \sum_{i=1}^n u_i \frac{\partial f_i}{\partial u_j}(tu)\, dt$$

sym.

$$= \int_0^1 f_j(tu) + t \sum_{i=1}^n u_i \frac{\partial f_j}{\partial u_i}(tu)\, dt$$

$$= \int_0^1 \frac{d}{dt}\left(t\, f_j(tu)\right) dt = f_j(u) \quad \square.$$

Recall Poincaré thm.

Hamiltonian dyn $\Longleftrightarrow$ symplecticity

integrability lemma.

<u>Thm</u>. $f: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. $f \in C^1$, $\dot{u} = f(u)$ w.
flow map $\varphi_t(u_0)$. φ_t is symplectic. then
there exists $H: \mathbb{R}^{2d} \to \mathbb{R}$ s.t.

$$f(u) = J^{-1} \nabla H(u), \quad \forall u \in \mathbb{R}^{2d}.$$