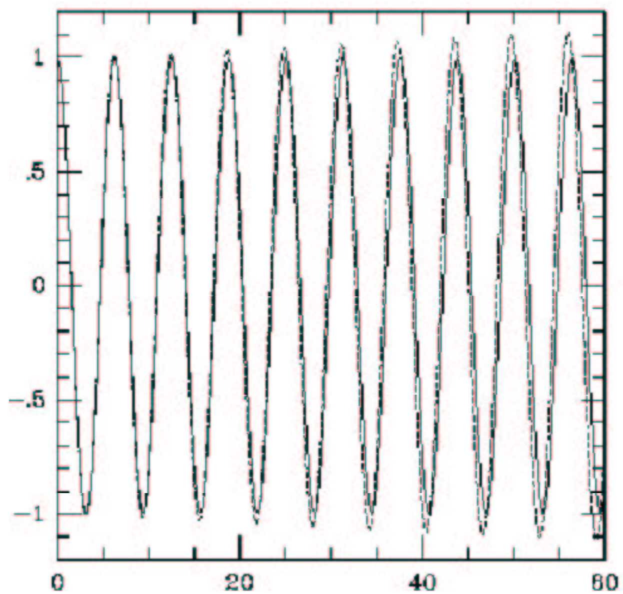
5. Integration method for Hamiltonian system.

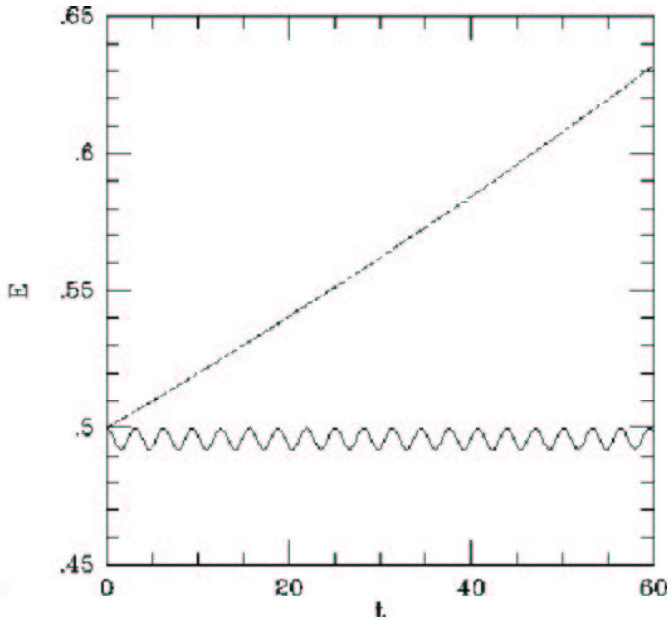
Consider the integration of Hamiltonian system in which the energy is conserved.

- In many of formulas (e.g. the classical RK4), the errors in conserved quantities (energy, angular momentum) accumulate in time.
- A numerical integration scheme that conserves the energy may be suitable for solving particular problems.

  ex) A long-term stability of the planetary system.
- Symplectic integration method and Symmetric integration method are known to have this property.

Numerical solution for the harmonic oscillator, $\frac{d^2x}{dt^2} = -kx$





- Comparison of 2nd order symplectic method and Runge-Kutta method

- Hamiltonian system has pure imaginary eigenvalue, $\dfrac{d^2x}{dt^2} = -kx \;\rightarrow\; \dfrac{dy}{dt} = \lambda y$
- When a stable numerical method is applied, an oscillatory solution often tends to be dumped or diverges.
- If the region of stability of the method includes the imaginary axis, the numerical solution oscillates correctly.

Cf.) Some methods suitable for 2nd order ODEs.

- Stormer-Cowell method.

$$\frac{d^2y}{dt^2} = f(t,y) \;\rightarrow\; \frac{w_{i+1} - 2w_i + w_{i-1}}{h^2} = \sum_{j=0}^{m} b_j f_{i+1-j}$$

Extremely high precision formulas $O(h^{14})$, $O(h^{16})$ are used in the celestial mechanics. Amount of floating operations, memory, are about a half of Adams methods.

Ex) Verlet Method : $w_{i+1} - 2w_i + w_{i-1} = h^2 f_i$

- Runge-Kutta-Nystroem method.

  Better accuracy for the same level RK formula, less memory.

Exc 5-1) Show that the Verlet method and leap flog method are the same.

Hamiltonian system.

q : coordinate of dynamical system. ($\dot{q} := \frac{dq}{dt}$.)

p : conjugate momentum. ($p := \frac{\partial L}{\partial \dot{q}}$. L : Lagrangian.)

Hamiltonian :

$$H(p,q) = T(p) + U(q)$$
$$(:= p\dot{q} - L)$$

Hamilton's equation.

$$\begin{cases} \dfrac{dq}{dt} = \dfrac{\partial H}{\partial p} \\ \dfrac{dp}{dt} = -\dfrac{\partial H}{\partial q} \end{cases}$$

Poisson bracket:

$$\{f,g\} := \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q}$$

$$\frac{d}{dt}f(p,q,t) = \frac{\partial f}{\partial t} - \{H,f\}$$

- Rewriting Hamilton's equation,

$$\frac{dy}{dt} = D_H\, y = \{y, H\}, \quad \text{where} \quad D_H := -\{H, \cdot\}, \quad y := \begin{pmatrix} p \\ q \end{pmatrix}$$

a formal solution is written $y(t) = \exp[tD_H]\, y(0)$.

The operator $\exp[tD_H]$ is well defined in the following sense;

$$\exp[tD_H] := \sum_{n=0}^{\infty} \frac{1}{n!}(t\, D_H)^n \quad \text{and since} \quad \frac{d}{dt}D_H\, y = D_H \frac{dy}{dt}$$

$$y(t+h) = \exp[hD_H]\, y(t) = \sum_{n=0}^{\infty} \frac{y^{(n)}(t)}{n!} h^n.$$

Symplectic formula.

- For the Hamiltonian $H(p,q) = T(p) + U(q)$, we have $D_H = D_T + D_U$.
- A symplectic map $\exp[hD_H] : y(t) \mapsto y(t+h)$ can be approximated by two subsequent symplectic maps $\exp[hD_T]$ and $\exp[hD_U]$;

$$\exp[hD_T] : y(t) \mapsto y(t+h) = \begin{pmatrix} q(t) + h\frac{\partial T}{\partial p} \\ p(t) \end{pmatrix}$$

$$\exp[hD_U] : y(t) \mapsto y(t+h) = \begin{pmatrix} q(t) \\ p(t) - h\frac{\partial U}{\partial q} \end{pmatrix}$$

$$\exp[hD_U]\exp[hD_T] : \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} \mapsto \begin{pmatrix} q(t+h) \\ p(t+h) \end{pmatrix} = \begin{pmatrix} q(t) + h\dfrac{\partial T}{\partial p}(t) \\ p(t) - h\dfrac{\partial U}{\partial q}(t+h) \end{pmatrix}$$

becomes 1st order symplectic formula.

cf) Theorem: (Liouville)
For a symplectic map, $\exp[tD_H] : y(0) \mapsto y(t)$,
the volume of phase space is invariant, $\int dq(0)dp(0) = \int dq(t)dp(t)$,
i.e Jacobian $\det M = 1$, where $M := \dfrac{\partial(q(t),p(t))}{\partial(q(0),p(0))}$,
or $MJM^\dagger = J$, where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$, I identity.

Exponential law for the non-commutative operators.

For non-comutative operators A and B, the exponential map $\exp[h(A+B)]$ can be decomposed into the infinite products

$$\exp[h(A+B)] = \lim_{k\to\infty} \prod_{i=1}^{k} \exp[a_i hA] \exp[b_i hB],$$

where a_i and b_i are constants.

- Symplectic integration formula approximate this infinite products by finite products as

$$\exp[h(A+B)] = \prod_{i=1}^{k} \exp[a_i hA] \exp[b_i hB] + O(h^{n+1}),$$

The number of product, k, is taken large enough to have a desirable order truncation error $O(h^{n+1})$.

(For this formula, the local truncation error is $\tau = O(h^n)$.)

Exc 5-2) Show that the 2nd order symplectic formula is the same as the Verlet method.

Exc 5-3) Check if the symplectic formulas generated by the symplectic maps $\exp[\frac{h}{2}D_T]\exp[hD_U]\exp[\frac{h}{2}D_T]$ and $\exp[\frac{h}{2}D_U]\exp[hD_T]\exp[\frac{h}{2}D_U]$

are the same.

Why the symplectic formula conserves energy?

Theorem : (Baker-Campbell-Hausdorff formula) Any finite products of two symplectic maps of non-comutative operators For non-comutative operators A and B, the exponential map $\exp[A] = e^A := \sum_{n=0}^{\infty} \frac{A^n}{n!}$, $\quad e^Z = e^A e^B$ is solved for the operator Z,

$$Z = \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sum_{\substack{r_i+s_i>0 \\ 1\leq i\leq n}} \frac{A^{r_1}B^{s_1}\cdots A^{r_n}B^{s_n}}{r_1!s_1!\cdots r_n!s_n!}$$

Therefore, for each symplectic formula, $\exists D$ such that

$$\exp[hD] = \prod_{i=1}^{k} \exp[a_i h D_T]\exp[b_i h D_U].$$

This means that the symplectic formula is associated with the Hamiltonian of the different dynamical system. $D = D_H + h^{p+1}D_{H_p} + O(h^{p+2})$ or
$H' = H + h^{p+1}H_p + O(h^{p+2})$. $H' \neq H$.

Exc 5-4) Integrate harmonic oscillator using some symplectic formulas, as well as the other non-symplectic formula of the same order.

Then compare the conservation of the energy in time.

Some systematic decomposition method for the exponential products.

$$\begin{aligned}\exp[h(D_T + D_U)] &= \prod_{i=1}^{k} \exp[a_i h D_T] \exp[b_i h D_U] + O(h^{n+1}) \\ &= S_n(h) + O(h^{n+1}).\end{aligned}$$

$$S_1(t) = \exp[hD_T] \exp[hD_U]$$

$$S_2(t) = \exp[\tfrac{h}{2} D_T] \exp[hD_U] \exp[\tfrac{h}{2} D_T]$$

(1) $S_n(h) = S_{n-1}(s_n h)\, S_{n-1}((1-s_n)h),$

where $s_n^n + (1-s_n)^n = 0, \quad s_n = \dfrac{1}{1+\exp(i\pi/n)}.$

(2) $S_n(h) = S_{n-1}(s_n h)\, S_{n-1}((1-2s_n)h)\, S_{n-1}(s_n h),$

where $2s_n^n + (1-2s_n)^n = 0, \quad s_n = \dfrac{1}{2-\sqrt[n]{2}}.$

(3) $S_n(h) = S_{n-1}(s_n h)\, S_{n-1}(s_n h)\, S_{n-1}((1-4s_n)h)\, S_{n-1}(s_n h)\, S_{n-1}(s_n h),$

where $4s_n^n + (1-4s_n)^n = 0, \quad s_n = \dfrac{1}{4-\sqrt[n]{4}}.$

Formulas (2) and (3) are symmetric, $S_n(h)\, S_n(-h) = 1$

Symplectic formula with symmetric decomposition.

Consider a relation between even (2n) and odd (2n-1) levels.

$$\exp[\,h(D_T + D_U)] = S_{2n-1}(h) + h^{2n} R_{2n}(D_T, D_U) + O(h^{2n+1}).$$

If $S_{2n-1}(h)$ is symmetric decomposition $S_{2n-1}(h)\,S_{2n-1}(-h) = 1$,

$$\begin{aligned}
&\exp[\,h(D_T + D_U)]\exp[\,-h(D_T + D_U)] = 1\\
&\quad = \left[\,S_{2n-1}(h) + h^{2n} R_{2n}(D_T, D_U) + O(h^{2n+1})\right]\\
&\qquad \times \left[\,S_{2n-1}(-h) + h^{2n} R_{2n}(D_T, D_U) + O(h^{2n+1})\right].\\
&\quad = 1 + h^{2n}\left[S_{2n-1}(h)\,R_{2n}(D_T, D_U) + R_{2n}(D_T, D_U) S_{2n-1}(-h)\right]\\
&\qquad + O(h^{2n+1}),
\end{aligned}$$

hence, $S_{2n-1}(h)\,R_{2n}(D_T, D_U) + R_{2n}(D_T, D_U) S_{2n-1}(-h) = O(h)$ for any h, that is, $R_{2n}(D_T, D_U) = 0$.

Formulas (2) and (3) becomes

(2) $S_{2n}(h) = S_{2n-1}(h) = S_{2n-2}(s_{2n-1}h)\,S_{2n-2}((1-2s_{2n-1})h)\,S_{2n-2}(s_{2n-1}h)$,

where $2s_m^m + (1-2s_m)^m = 0, \quad s_m = \dfrac{1}{2-\sqrt[m]{2}}.$

(3) $S_{2n}(h) = S_{2n-1} = [S_{2n-2}(s_{2n-1}h)]^2\,S_{2n-2}((1-4s_{2n-1})h)\,[S_{2n-2}(s_{2n-1}h)]^2$,

where $4s_m^m + (1-4s_m)^m = 0, \quad s_m = \dfrac{1}{4-\sqrt[m]{4}}.$

Symmetric integration formulas

A few drawback of the symplectic formula

– Difficult to change the time step size h.

Once change the step size, the formula is no more symplectic.

– floating operation is way more than the multistep method of comparable order.

⋆ The one-step method for the 1st order ODE, $\frac{dy}{dt} = f(t,y)$,

$w_{i+1} = \phi(t_i, w_i, f, h)$ is time symmetric if $w_i = \phi(t_{i+1}, w_{i+1}, -f, h)$.

Ex) Trapezoidal formula

⋆ The multistep method for the 2nd order ODE, $\frac{d^2y}{dt^2} = f(t,y)$,

$\sum_{j=0}^{m} a_j w_{i+1-j} = h^2 \sum_{j=0}^{m} b_j f_{i+1-j}$ is time symmetric,

if $a_i = a_{m-i}$ and $b_i = b_{m-i}$ for $i = 1, \cdots, m$ are satisfied.

Symmetric formula

– the error in the energy is bounded similar to symplectic formula.

– No difficulty in changing the time step size h.

Symmetric integration formulas (continue)

⋆ Hermite type formula – combines Hermite interpolation formula and Taylor's method.

The 2nd order Taylor: $w_{i+1} = w_i + hf(t_i, w_i) + \frac{h^2}{2}\frac{df}{dt}(t_i, w_i)$.

The 2nd order Hermite: $w_{i+1} = w_i + \frac{h}{2}(f_i + f_{i+1}) + \frac{h^2}{12}(f_i' - f_{i+1}')$.

– An implicit formula. Symmetric.

– Direct iteration can be used.

– relatively simple coding and decent accuracy.

Exc 5-5) Derive the above 2nd order Hermite formula

– Method for changing step size in symmetric formula.

– Stability of symmetric formula – linear stability and P-stability.