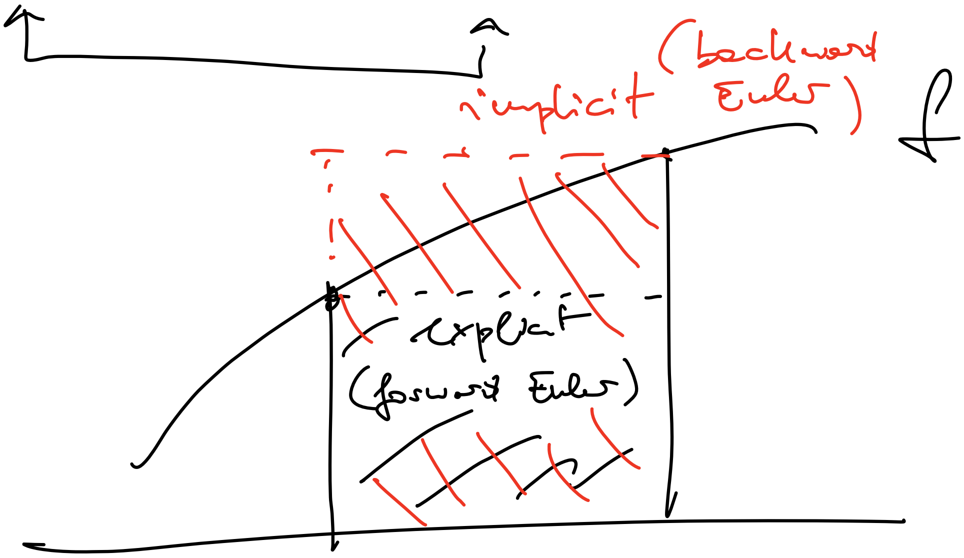
Numerical solution of ODEs

⊙ Stiff ODEs and implicit methods

$$\vec{y}_{n+1} = \mathcal{Y}_n\left(\vec{y}_{n+1}, \vec{y}_n, \dots, \vec{y}_0 ; \vec{f}, \underline{h}\right)$$



"Stiffness"

method convergent of order p

$$\| \vec{y}(t_n) - \vec{y}_n \| \overset{h \to 0}{\sim} o(h^p) = A h^p = \left(\frac{h}{h_0}\right)^{p}$$

Forward Euler : $\alpha = \frac{h}{h_0}$

$h_0 \ll 1 \longrightarrow$ stiffness

Example

$\rightarrow \quad \dot{y} = -ay \qquad a > 0$

$y(t) = y_0 e^{-at} \qquad y(0) = y_0$

forward Euler :

$$y_{n+1} = y_n + h f(y_n)$$

$$= y_n - h a y_n = y_n (1 - ha)$$

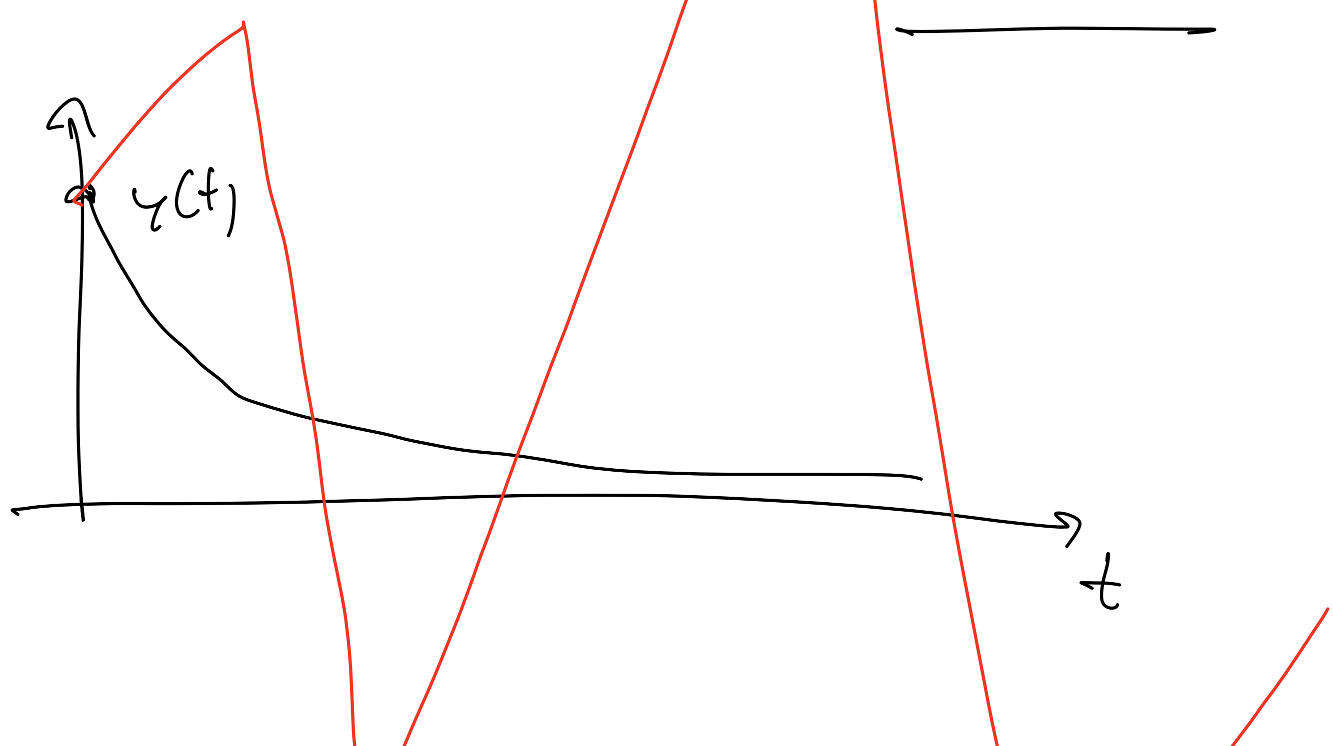
$$= \ldots = (1 - ha)^{n+1} y_0$$

$|1 - ha| > 1$

$1 - ha < -1$

$ha > 2$

$h > \frac{2}{a} = h_0$



Backward Euler

$$y_{n+1} = y_n - ha\, y_{n+1}$$

$$y_{n+1} = \frac{y_n}{1+ha} = \dots = \frac{y_0}{(1+ha)^{n+1}}$$

$1+ha > 1 \quad \forall h$

A-stability (absolute stability)

reference Cauchy problem

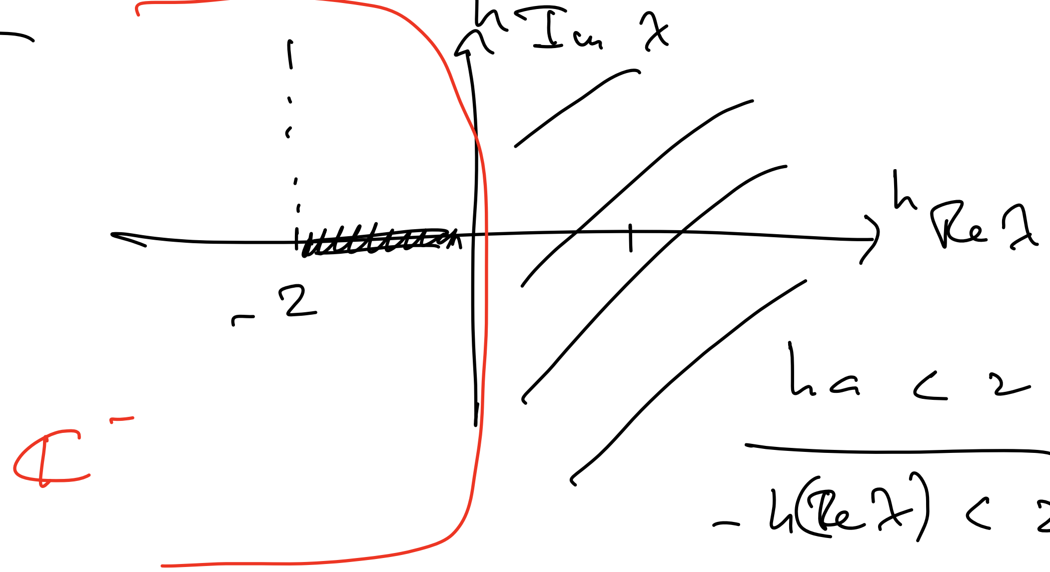
$$\begin{cases} \dot{y} = \lambda y \\ y(0) = y_0 \end{cases} \qquad \lambda \in \mathbb{C} \quad (y \in \mathbb{C})$$

Numerical method $\rightarrow$ linear stability domain $(\mathcal{D})$ ✓

set of values of $h\lambda = z \in \mathbb{C}$:

$\rightarrow$ $y_n \xrightarrow[n\to\infty]{} 0$

$$\mathcal{D}_{\text{Forw. Euler}} = \{ h\lambda \in \mathbb{C} \,|\, |1+h\lambda| < 1 \}$$



$$ha < 2$$

$$-h(\mathrm{Re}\,\lambda) < 2$$

$$\mathcal{D}_{\text{Back. Euler}} = \{ h\lambda \in \mathbb{C} \mid |1-h\lambda| < 1 \}$$

$$\sqrt{(1-\mathrm{Re}\,\lambda)^2 + (\mathrm{Im}\,\lambda)^2} < 1$$

$$\Rightarrow \underline{\mathrm{Re}\,\lambda < 0}$$

$$\mathbb{C}^- \subseteq \mathcal{D}_{\text{Back. Euler}}$$

$$\boxed{\underline{\text{A-stability}} \text{ of a method} : \quad \mathbb{C}^- \subseteq \mathcal{D}}$$

<u>Facts</u>

⇒ No explicit RK method is A-stable

→ Gauss-Legendre RK methods are all A-stable

$$\begin{cases} \text{order-1} & : \text{backward Euler} \\ \text{order-2} & : \text{implicit mid-point} \end{cases}$$

...

Backward Euler

$$\vec{y}_{n+1} = \vec{y}_n + h \, \vec{f}(\vec{y}_{n+1}, t_{n+1})$$

error of order $O(h^2)$

Predictor - corrector method

predictor step : Forward Euler

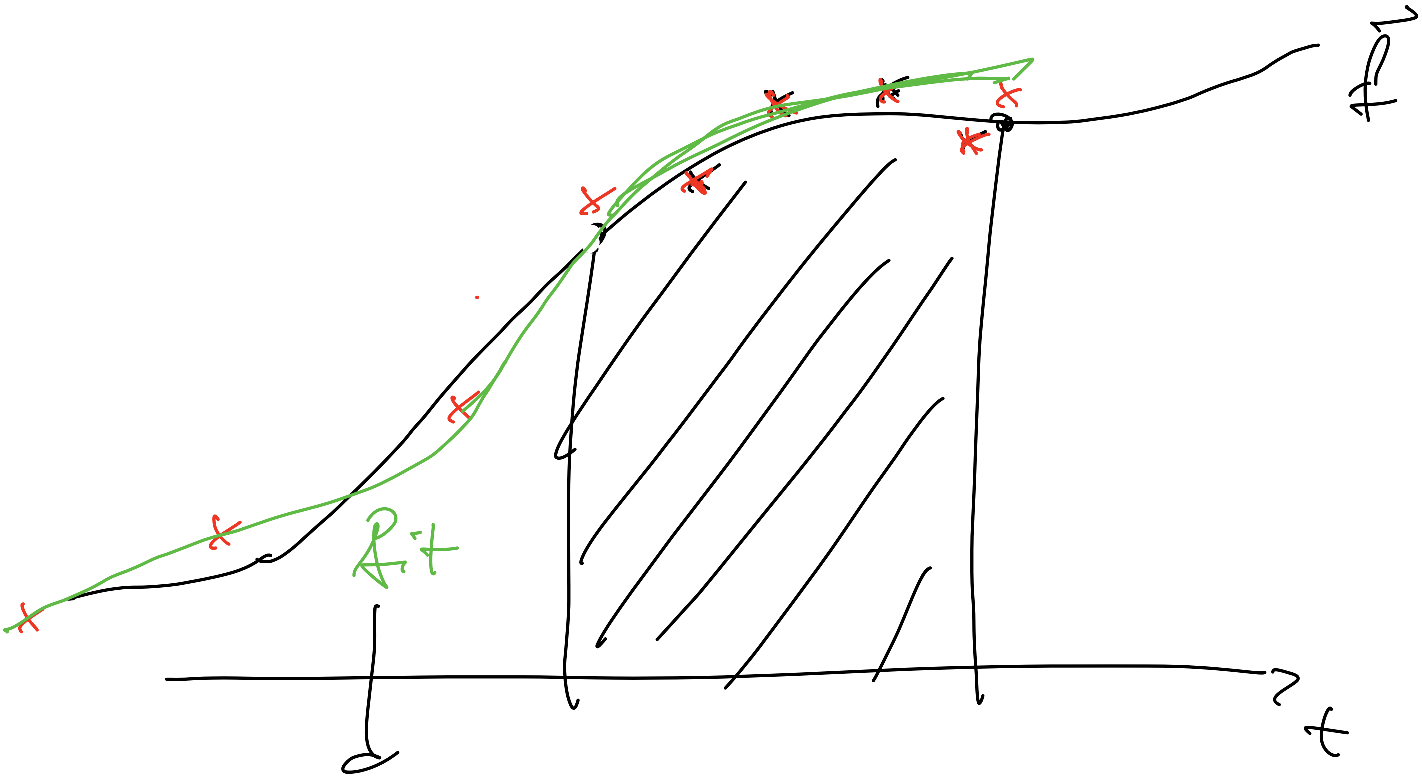
$$\vec{y}_n \to \underbrace{\vec{y}_{n+1}^{(0)}} = \vec{y}_n + h\vec{f}(\underline{\vec{y}_n}, t_n)$$

corrector step

$$\vec{y}_{n+1}^{(1)} = \vec{y}_n + h \, \vec{f}(\vec{y}_{n+1}^{(0)}, t_{n+1})$$

$$= \vec{y}_n + h \vec{f}(\vec{y}_{n+1}^{(1)}, t_n) + O(h^2)$$

Multi-step methods



polynomial fit of previously calculated points

Adams-Bashforth (s-step)

$$\vec{y}_{n+1} = \vec{y}_n + h \sum_{m=0}^{s-1} b_m \vec{f}(\vec{y}_{n-m}, t_{n-m})$$

ex.

$s=2$

$$\vec{y}_{n+1} = \vec{y}_n + h\left[\frac{3}{2}\vec{f}(\vec{y}_n, t_n) - \frac{1}{2}\vec{f}(\vec{y}_{n-1}, t_{n-1})\right]$$

→ A-stability : the highest order of an A-stable multi-step method is $p = 2$.

(2^{nd} Dahlquist barrier)

→ There are no multi-step methods which are symplectic.

Symplectic integration methods

Hamilton equations

$(\vec{p}_1, \vec{q}_1)$

$(\vec{p}_2, \vec{q}_2)$

...

$\vec{p} = (\vec{p}_1, \vec{p}_2, \dots, \vec{p}_N)$

$\vec{q} = (\vec{q}_1, \vec{q}_2, \dots, \vec{q}_N)$

$\in \mathbb{R}^{3N}$

$H = H(\vec{p}, \vec{q})$

$$\begin{cases} \dot{\vec{p}} = -\nabla_{\vec{q}} H(\vec{p}, \vec{q}) \\ \dot{\vec{q}} = \nabla_{\vec{p}} H(\vec{p}, \vec{q}) \end{cases}$$

$\vec{z} = (\vec{p}, \vec{q})$

$$\vec{\nabla}_{\vec{z}} \mathcal{H} = \left(\vec{\nabla}_{\vec{p}} \mathcal{H}, \ \vec{\nabla}_{\vec{q}} \mathcal{H} \right)$$

$$\dot{\vec{z}} = J \, \vec{\nabla}_{\vec{z}} \mathcal{H}$$

$$J = \left(\begin{array}{c|c} 0 & -\mathbb{1}_{3N} \\ \hline \mathbb{1}_{3N} & 0 \end{array} \right)$$

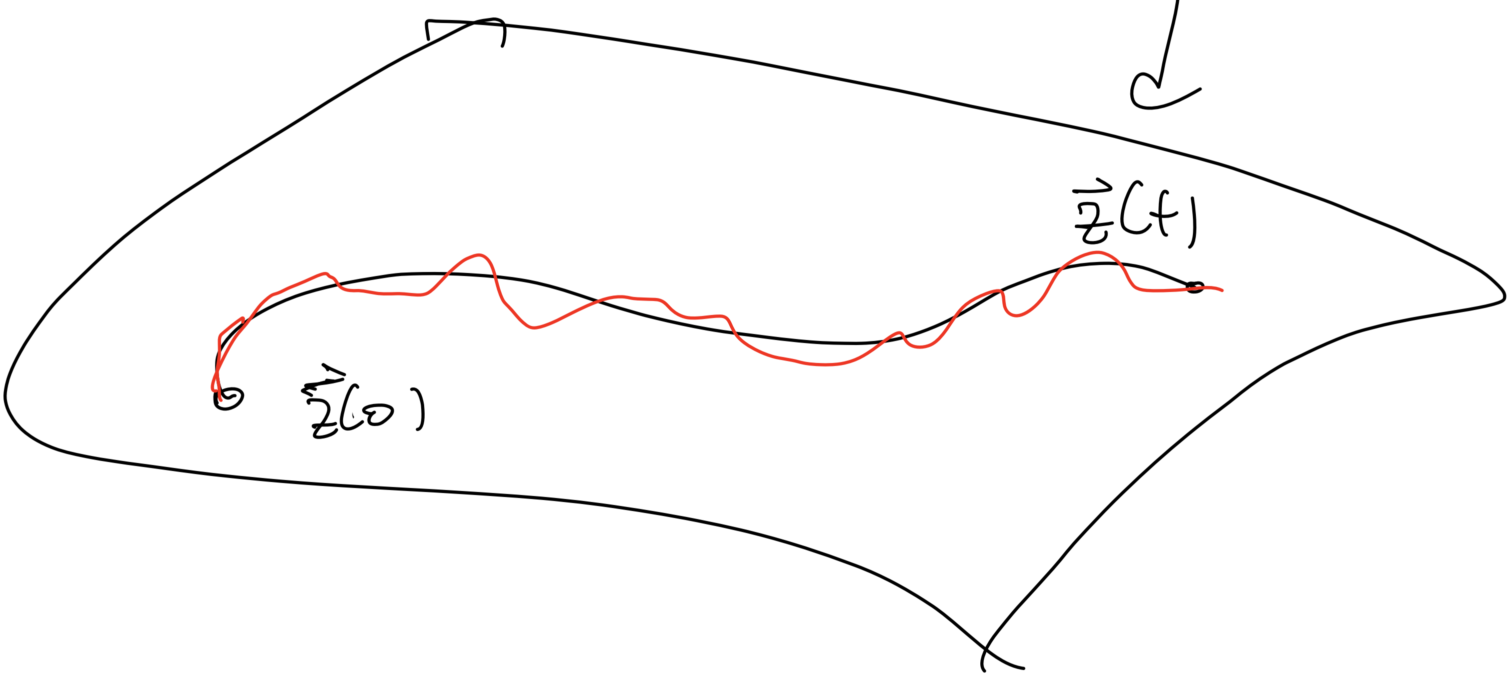
$$\frac{d}{dt} \Big[\mathcal{H} (\overbrace{\vec{p}(t), \vec{q}(t)}^{\vec{z}(t)}) \Big] = 0$$

$$\vec{\vartheta}_t : \ \vec{z}(0) \in \mathbb{R}^{6N} \longrightarrow \vec{z}(t) \in \mathbb{R}^{6N}$$

map (Hamiltonian flow)

$$\vec{\vartheta}_t [z(0)] = \vec{z}(t)$$

$$\mathcal{H}[z(t)] = \text{const.}$$



Symplectic structure of Hamilton flow

infinitesimal Hamilton flow

$$\vec{z}(t+h) = \left(\mathbb{1} + h\, J\, \vec{\nabla}_{\vec{z}} \mathcal{H}(\cdot,\cdot)\right) \vec{z}(t)$$

$$\dot{\vec{z}}(t) = J\, \vec{\nabla}_{\vec{z}} \mathcal{H}[\vec{z}(t)]$$

$$= \vec{z}(t) + h\, J\, \nabla_{\vec{z}} \mathcal{H}[\vec{z}(t)] + \dots$$

$$\vec{\varphi} : \vec{z} \in \mathbb{R}^{6N} \to \vec{z}\,' = J\, \vec{\nabla}_{\vec{z}} \mathcal{H}[\vec{z}] \in \mathbb{R}^{6N}$$

Jacobian matrix of the map

$$L = \frac{\partial \vec{\varphi}}{\partial \vec{z}} = \frac{\partial}{\partial \vec{z}} \left[J\, \vec{\nabla}_{\vec{z}} \mathcal{H} \right] =$$

$$= J \left\{ \frac{\partial^2 \mathcal{H}}{\partial z_i \partial z_j} \right\}$$

$$= \dots = \begin{pmatrix} -\mathcal{H}_{qp} & -\mathcal{H}_{qq} \\ \mathcal{H}_{pp} & \mathcal{H}_{pq} \end{pmatrix}$$

$$\mathcal{H}_{qp} = \left\{ \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_j} \right\} = \mathcal{H}_{pq}$$

$$\boxed{L^T J + J L = 0}$$

Full Hamilton flow

formal solution

$$\vec{\phi}_t : \vec{z}(0) \longrightarrow \vec{z}(t) = \underbrace{\exp\left(t\, J \vec{\nabla}_{\vec{z}} \mathcal{H}\right)}[\vec{z}(0)]$$

$$\dot{\vec{z}}(t) = J \underbrace{\vec{\nabla}\mathcal{H}}[\vec{z}(t)]$$

$$= \underbrace{\sum_{n=0}^{\infty} \frac{t^n}{n!} J \overbrace{\vec{\nabla}\mathcal{H}[\vec{\nabla}\mathcal{H}[\vec{\nabla}\mathcal{H}[\ldots[\vec{z}(0)]]\ldots]}^{n \text{ times}}}$$

Jacobian matrix

$$S = \frac{\partial \vec{\phi}_t}{\partial \vec{z}} = e^{tL}$$

$$\boxed{S^T J S = J}$$

S symplectic matrix

orthogonal matrix $O^T \mathbb{1}\, O = \mathbb{1}$

<u>Numerical method</u> : <u>also a map ?</u>

$$\vec{y}_{n+1} = \vec{\phi}_{t}(\vec{y}_n)$$

map

$\vec{\vartheta}_f : \quad \vec{y}_n \longrightarrow \vec{y}_{n+1} = \vec{\vartheta}(\vec{y}_n)$

Jacobian matrix $\quad \dfrac{\partial \vec{\vartheta}}{\partial \vec{z}}$

if symplectic

$\Rightarrow$ symplectic method

RK methods

$$\begin{array}{c|cccc} b_1 & a_{11} & a_{12} & - & \\ b_2 & \vdots & & & \\ \vdots & & & & \\ b_m & & & & \\ \hline & c_1 & c_2 & - & c_m \end{array}$$

$$\{ b_k, c_k, a_{kl} \}$$

matrix M

$$M_{kl} = b_k a_{kl} + b_l a_{lk} - b_k b_l$$

if $M = 0 \longrightarrow$ symplectic RK method

Ex.: implicit midpoint rule

method as a

symplectic map $\rightarrow$ Hamilton equations

$$\vec{z}_{n+1} = \exp[h \, \vec{\nabla} \tilde{H}](\vec{z}_n)$$

$\tilde{\mathcal{H}}$ = conserved

$\tilde{\mathcal{H}} \simeq \mathcal{H}$

Building symplectic integrators

$$\mathcal{H}(\vec{p}, \vec{q}) = \underset{\text{kinetic}}{T(\vec{p})} + \underset{\text{potential}}{U(\vec{q})}$$

$$\dot{\vec{z}} = J \vec{\nabla}_{\vec{z}} \mathcal{H} = J\left(-\nabla_{\vec{q}} U, \ \nabla_{\vec{p}} T\right)$$

$$= \vec{Q}[\vec{z}] + \vec{R}[\vec{z}]$$

$$\begin{cases} \vec{Q}[\vec{z}] = (0, \nabla_{\vec{p}} T)[\vec{z}] \\ \vec{R}[\vec{z}] = (-\vec{\nabla}_{\vec{q}} U, 0)[\vec{z}] \end{cases}$$

$$\vec{z}(t) = \exp(t\, J \vec{\nabla} \mathcal{H})[\vec{z}(0)]$$

$$= \exp(t(\vec{Q} + \vec{R}))[\vec{z}(0)]$$

$$\vec{Q}[\vec{R}[\vec{z}]] \neq \vec{R}[\vec{Q}[\vec{z}]]$$

$t = h$

$$\boxed{e^{h(\vec{Q}+\vec{R})} \simeq e^{h\vec{Q}} e^{h\vec{R}} + o(h^2)}$$

$$e^{h(\vec{Q}+\vec{R})} = e^{h\vec{Q}/2}\, e^{h\vec{R}}\, e^{\frac{h}{2}\vec{Q}} + O(h^3)$$

...

$$e^{h\vec{Q}} \simeq \left(\mathbb{1} + h\vec{Q} + O(h^2)\right)$$

$$\vec{Z}_{n+1} \simeq (\mathbb{1} + h\vec{Q})(\mathbb{1} + h\vec{R})\,\vec{Z}_n$$

symplectic integrator

$$\begin{cases} \vec{p}_{n+1} = \vec{p}_n - h\,\vec{\nabla}_q U(\vec{q}_n) \\ \vec{q}_{n+1} = \vec{q}_n + h\,\vec{\nabla}_{\vec{p}} T(\vec{p}_{n+1}) \end{cases}$$

Verlet's scheme (order-1)

Störmer-Verlet (order 2)