

Geometric properties of exponentially fitted methods

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Exponentially fitted methods

In the past 15 years, our research group has constructed modified versions of well-known

- linear multistep methods
- Runge-Kutta methods

Aim : build methods which perform very good when the solution has a known exponential or trigonometric behaviour.

Linear multistep methods

Well known methods to solve

$$\ddot{q} = f(q(t)) \quad q(a) = q_a \quad \dot{q}(a) = \dot{q}_a$$

are

- Störmer-Verlet method (order 2)

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n)$$

- Numerov method (order 4)

$$q_{n+1} - 2q_n + q_{n-1} = \frac{h^2}{12} (f(q_{n-1}) + 10f(q_n) + f(q_{n+1}))$$

Construction

$$q(t_{n+1}) - 2q(t_n) + q(t_{n-1}) = \int_{t_n}^{t_{n+1}} (t_{n+1} - \tau) [\ddot{q}(\tau) + \ddot{q}(2t_n - \tau)] d\tau$$

- Störmer-Verlet

Replace $\ddot{q}(t) = f(q(t))$ by the interpolating polynomial

$p(t) = a_0 + a_1 t$ at t_n, t_{n+1} :

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n)$$

- Numerov

Replace $\ddot{q}(t) = f(q(t))$ by the interpolating polynomial

$p(t) = a_0 + a_1 t + a_2 t^2$ at t_{n-1}, t_n, t_{n+1} :

$$q_{n+1} - 2q_n + q_{n-1} = \frac{h^2}{12} (f(q_{n-1}) + 10f(q_n) + f(q_{n+1}))$$

Exponential fitting

Consider the initial value problem

$$\ddot{q} + \omega^2 q = g(q) \quad q(a) = q_a \quad \dot{q}(a) = \dot{q}_a .$$

If $|g(q)| \ll |\omega^2 q|$ then

$$q(t) \approx \alpha \cos(\omega t + \phi)$$

To mimic this oscillatory behaviour, one could replace polynomial interpolation by trigonometric interpolation
(in the complex case : exponential interpolation).

$$\text{Replace } p(t) = \sum_{i=0}^n c_i t^i \text{ by } p(t) = a \cos \omega t + b \sin \omega t + \sum_{i=0}^{n-2} c_i t^i .$$

Störmer-Verlet method

$$q(t_{n+1}) - 2q(t_n) + q(t_{n-1}) = \int_{t_n}^{t_{n+1}} (t_{n+1} - \tau) [\ddot{q}(\tau) + \ddot{q}(2t_n - \tau)] d\tau$$

Replace $\ddot{q}(t) = f(q(t))$ by an interpolating function $p(t)$ at t_n, t_{n+1} .

- classical : $p(t) = a_0 + a_1 t$

$$p(t) = \frac{t_{n+1} - t}{h} f_n + \frac{t - t_n}{h} f(q_{n+1})$$

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f_n$$

- exponentially fitted : $p(t) = a \cos \omega t + b \sin \omega t$

$$p(t) = \frac{\sin \omega(t_{n+1} - t)}{\sin \omega h} f_n + \frac{\sin \omega(t - t_n)}{\sin \omega h} f(q_{n+1})$$

$$q_{n+1} - 2q_n + q_{n-1} = h^2 \text{sinc}^2 \nu f(q_n) \quad \nu = \frac{\omega h}{2}$$

$$\text{sinc } x = \begin{cases} \frac{\sin x}{x} & x \neq 0 \\ 1 & x = 0 \end{cases} \quad \text{tanc } x = \begin{cases} \frac{\tan x}{x} & x \neq 0 \\ 1 & x = 0 \end{cases}$$

Numerov method

$$q(t_{n+1}) - 2q(t_n) + q(t_{n-1}) = \int_{t_n}^{t_{n+1}} (t_{n+1} - \tau) [\ddot{q}(\tau) + \ddot{q}(2t_n - \tau)] d\tau$$

Replace $\ddot{q}(t) = f(q(t))$ by an interpolating function $p(t)$ at t_{n-1} , t_n ,
 t_{n+1} .

- classical : $p(t) = a_0 + a_1 t + a_2 t^2$

$$q_{n+1} - 2q_n + q_{n-1} = h^2 (\lambda f(q_{n-1}) + (1 - 2\lambda) f(q_n) + \lambda f(q_{n+1}))$$

$$\lambda = \frac{1}{12}$$

- exponentially fitted : $p(t) = a \cos \omega t + b \sin \omega t + c_0$

$$q_{n+1} - 2q_n + q_{n-1} = h^2 (\lambda f(q_{n-1}) + (1 - 2\lambda) f(q_n) + \lambda f(q_{n+1}))$$

$$\lambda = \frac{1}{4} \left(\frac{1}{\sin^2 \nu} - \frac{1}{\nu^2} \right) = \frac{1}{12} + \frac{1}{60} \nu^2 + \frac{1}{378} \nu^4 + \dots \quad \nu = \frac{\omega h}{2}$$

Choice of ω

based on local truncation error

- Störmer-Verlet

$$y(x_{n+1}) - y_{n+1} = \frac{h^4}{12} \left(y^{(4)}(x_n) + \omega^2 y^{(2)}(x_n) \right) + \dots$$

$$\implies \omega_n^2 = -\frac{y^{(4)}(x_n)}{y^{(2)}(x_n)}$$

- Numerov

$$y(x_{n+1}) - y_{n+1} = -\frac{h^6}{240} \left(y^{(6)}(x_n) + \omega^2 y^{(4)}(x_n) \right) + \dots$$

$$\implies \omega_n^2 = -\frac{y^{(6)}(x_n)}{y^{(4)}(x_n)}$$

local optimization

The Störmer-Verlet method

Geometric numerical integration
illustrated by the Störmer Verlet method

E. Hairer, C. Lubich, G. Wanner

Acta Numerica (2003) 1–51

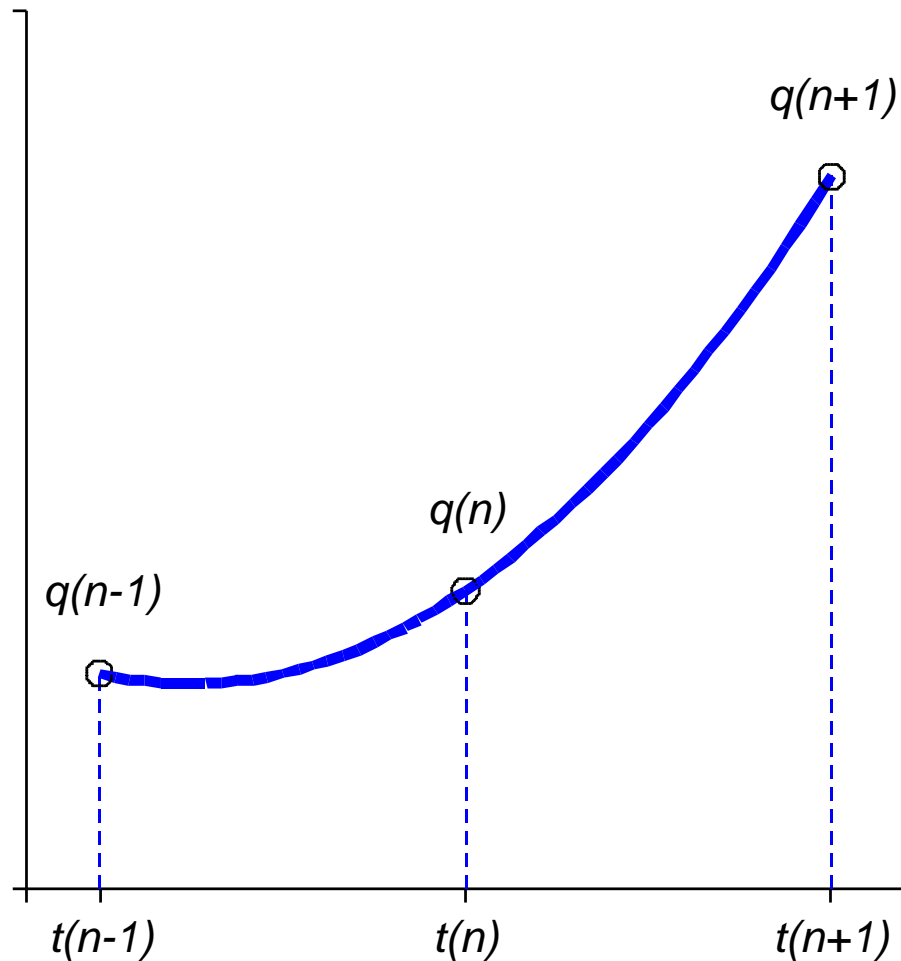
The Störmer-Verlet method

- construction

S/V : $q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n)$

Interpolate $q(t)$ by $p(t) = at^2 + bt + c$ at t_{n-1} , t_n and t_{n+1} .

Approximate $\ddot{q}(t_n) = f(q(t_n))$ by $\ddot{p}(t_n) = \frac{q_{n+1} - 2q_n + q_{n-1}}{h^2}$

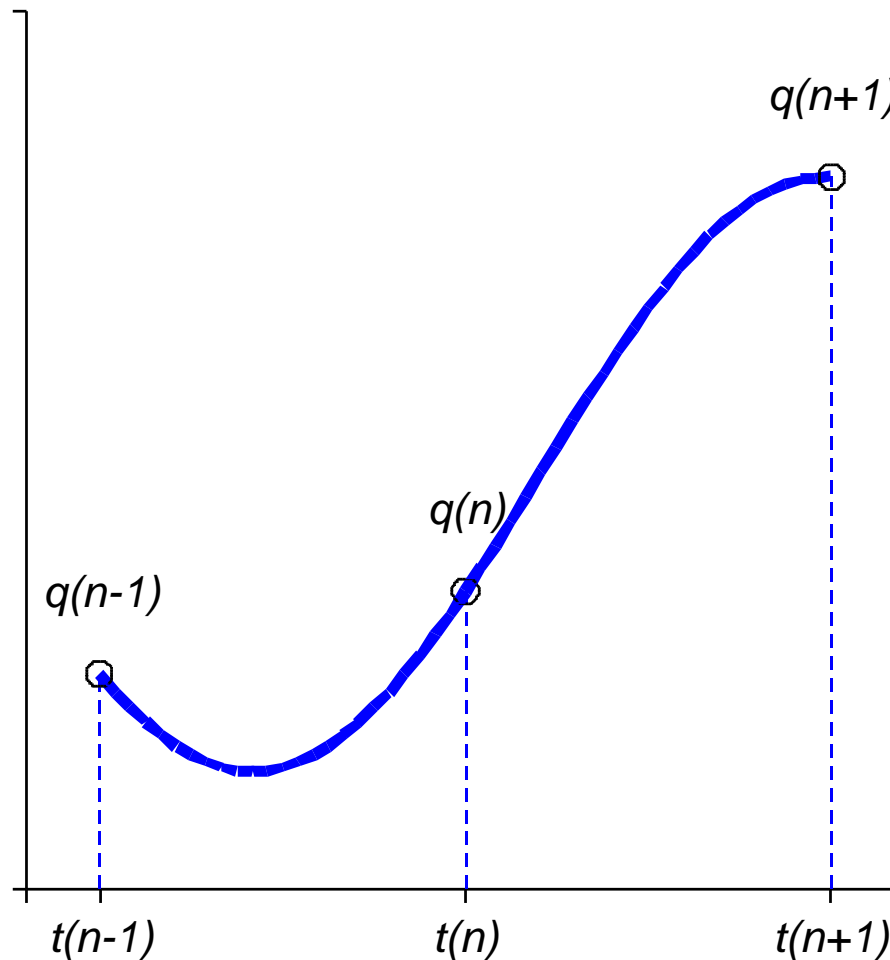


S/V_{EF}:

$$q_{n+1} - 2q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu f_n$$

Interpolate $q(t)$ by $p(t) = a \cos \omega t + b \sin \omega t + c$ at t_{n-1} , t_n and t_{n+1} .

Approximate $\ddot{q}(t_n) = f(q(t_n))$ by $\ddot{p}(t_n) = \frac{q_{n+1} - 2q_n + q_{n-1}}{h^2 \operatorname{sinc}^2 \nu}$



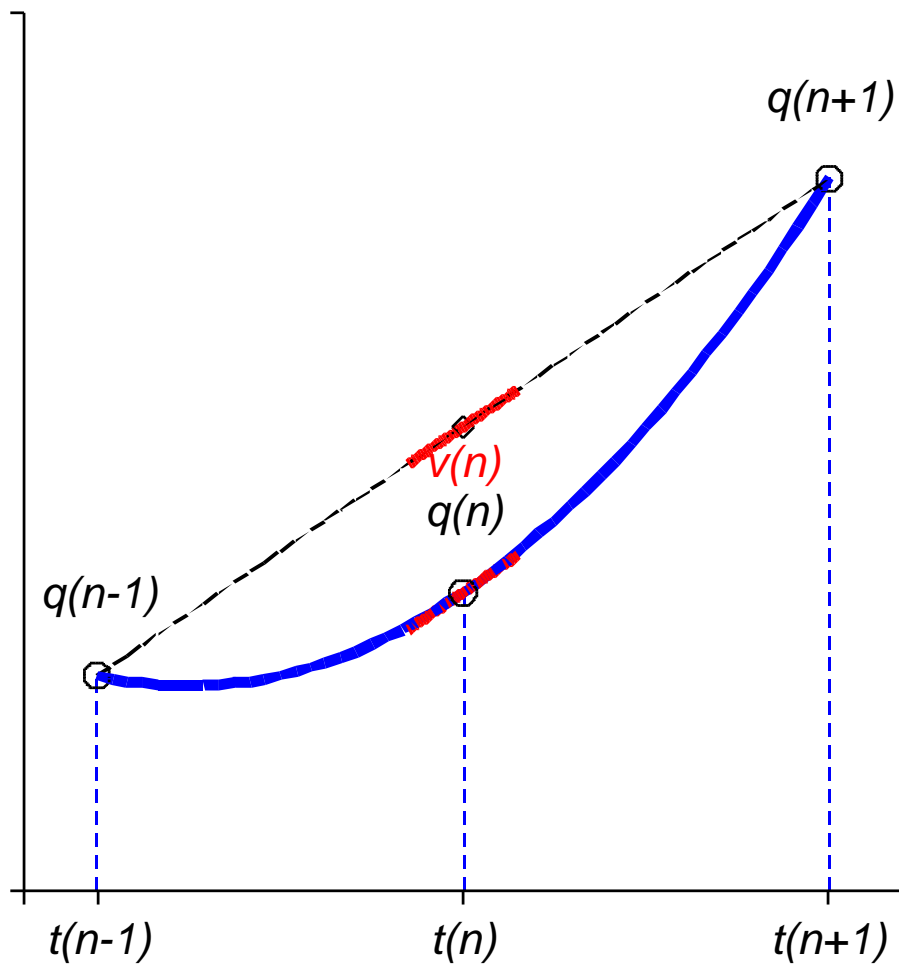
The Störmer-Verlet method

- construction
- one-step formulation

S/V : $q_{n+1} - 2q_n + q_{n-1} = h^2 f_n$

$$\dot{q} = v \quad \dot{v} = f(q)$$

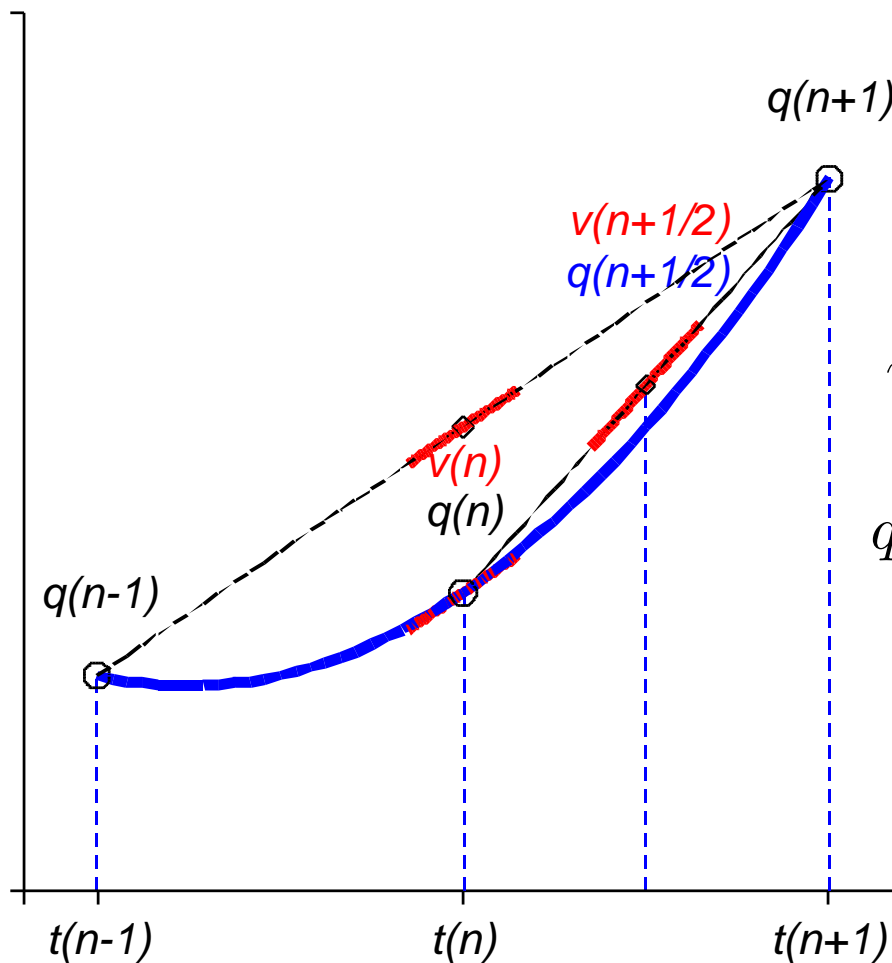
$$v(t_n) \approx \dot{p}(t_n) = \frac{q_{n+1} - q_{n-1}}{2h}$$



S/V : $q_{n+1} - 2q_n + q_{n-1} = h^2 f_n$

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$v(t_n) \approx \dot{p}(t_n) = \frac{q_{n+1} - q_{n-1}}{2h}$$



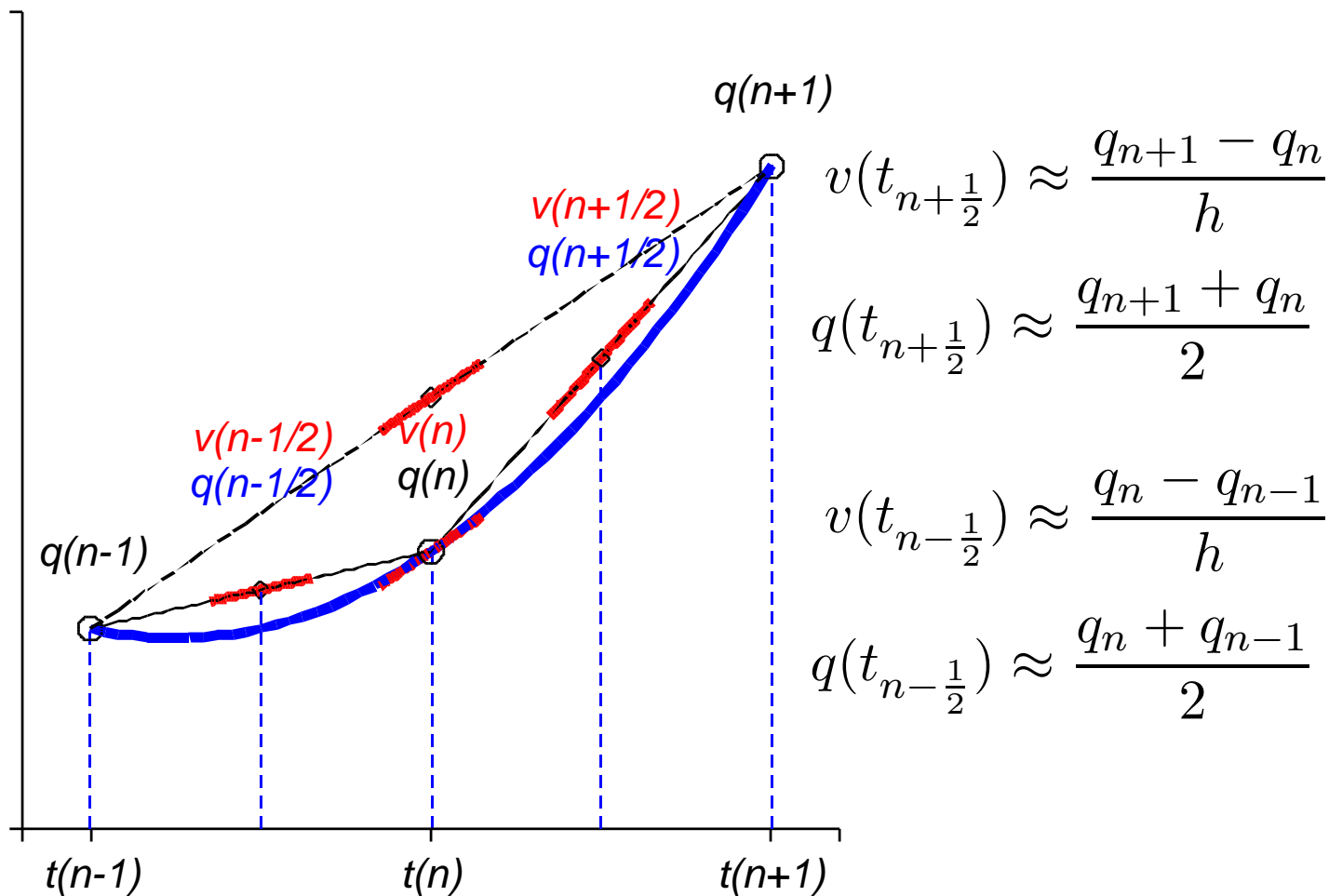
$$v(t_{n+\frac{1}{2}}) \approx \frac{q_{n+1} - q_n}{h}$$

$$q(t_{n+\frac{1}{2}}) \approx \frac{q_{n+1} + q_n}{2}$$

S/V : $q_{n+1} - 2q_n + q_{n-1} = h^2 f_n$

$$\dot{q} = v \quad \dot{v} = f(q)$$

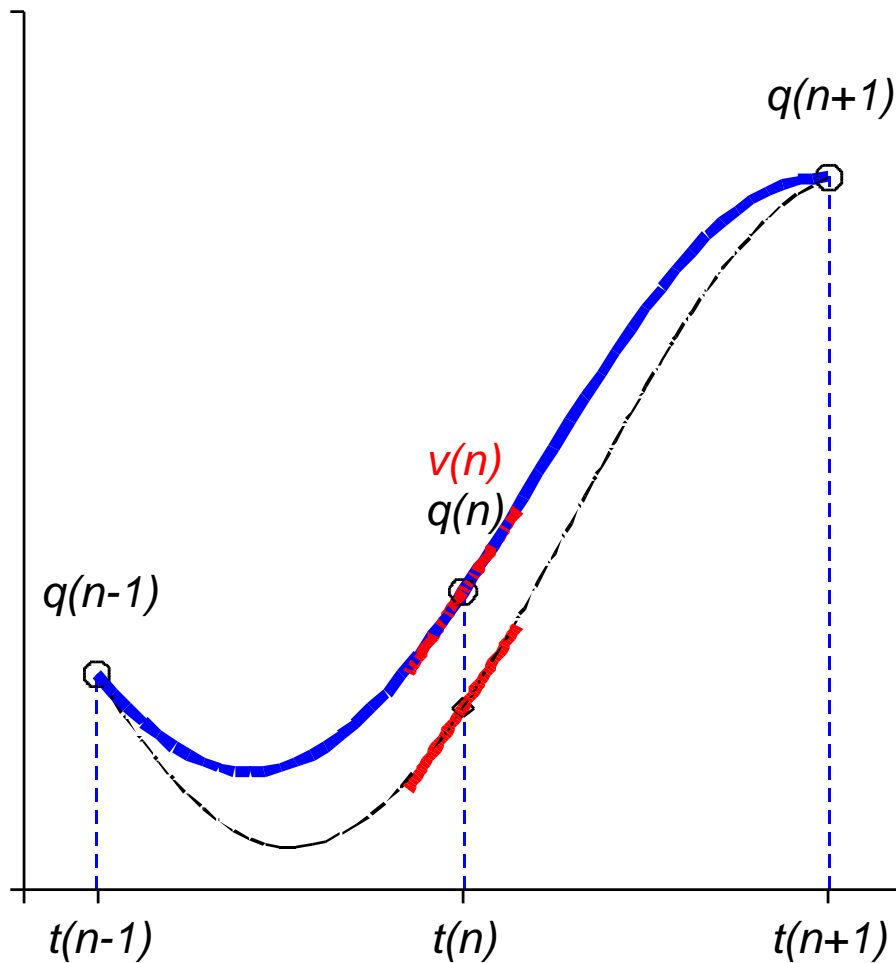
$$v(t_n) \approx \dot{p}(t_n) = \frac{q_{n+1} - q_{n-1}}{2h}$$



S/V_{EF}: $q_{n+1} - 2q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu f_n$

$$\dot{q} = v \quad \dot{v} = f(q)$$

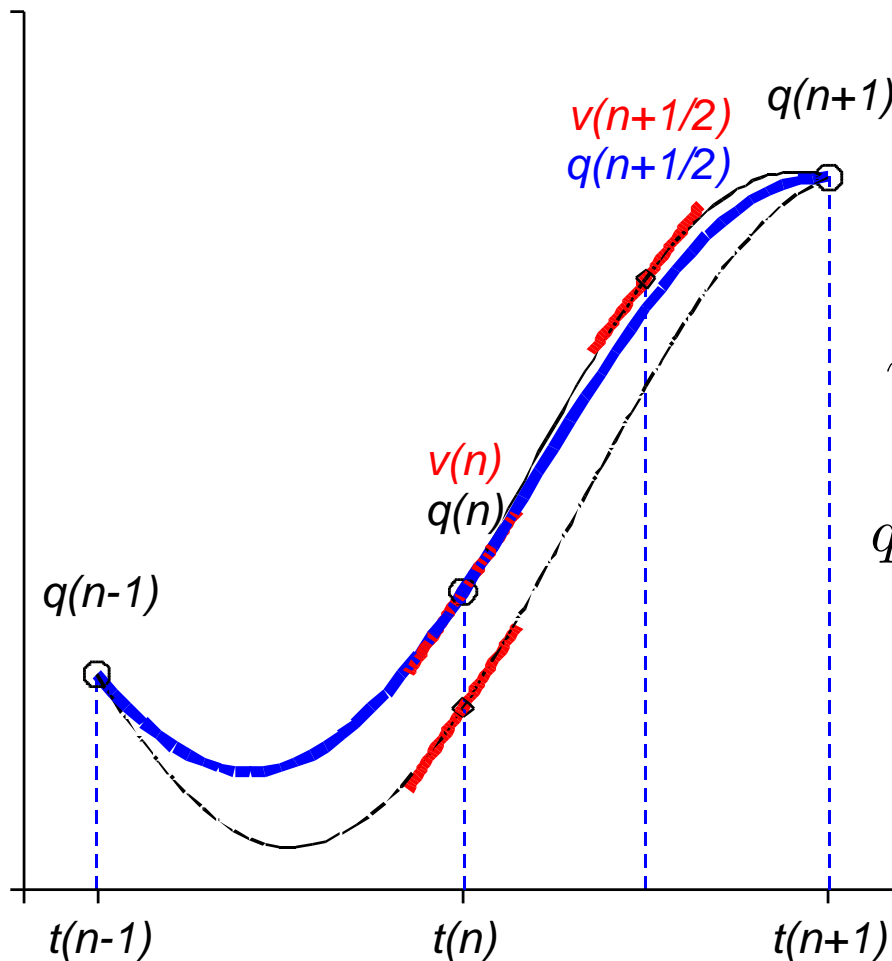
$$v(t_n) \approx \dot{p}(t_n) = \frac{1}{\operatorname{sinc} 2\nu} \frac{q_{n+1} - q_{n-1}}{2h}$$



S/V : $q_{n+1} - 2q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu f_n$

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$v(t_n) \approx \dot{p}(t_n) = \frac{1}{\operatorname{sinc} 2\nu} \frac{q_{n+1} - q_{n-1}}{2h}$$



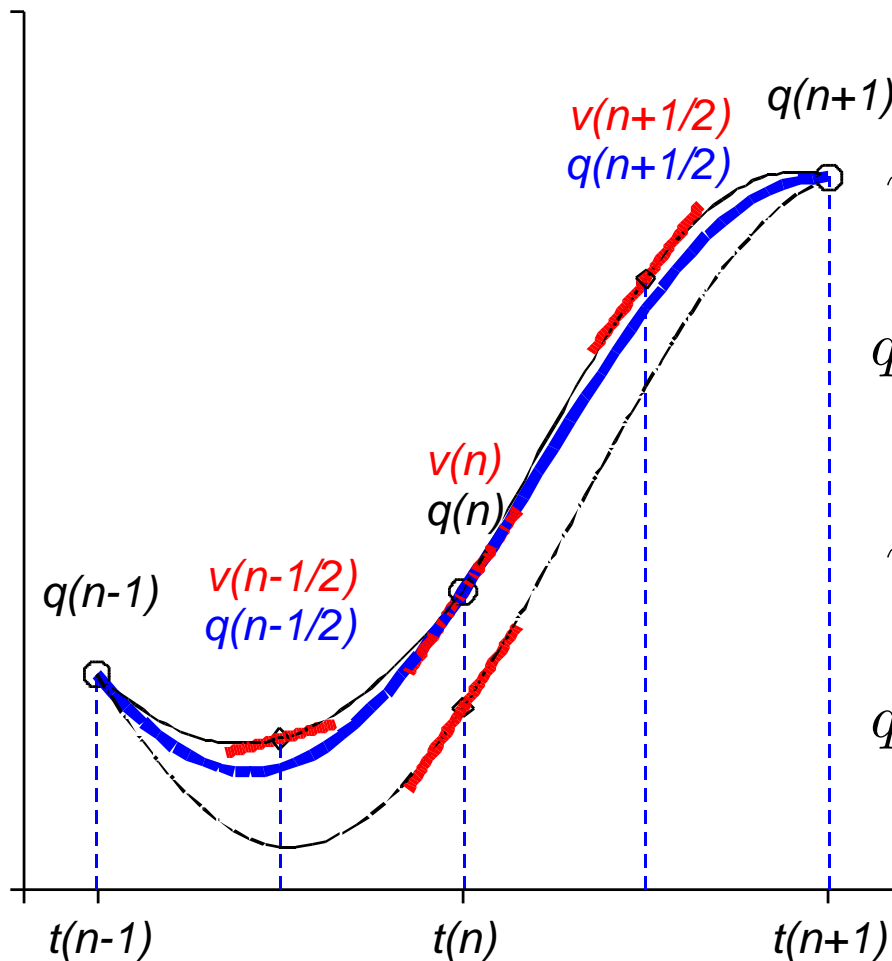
$$v(t_{n+\frac{1}{2}}) \approx \frac{1}{\operatorname{sinc} \nu} \frac{q_{n+1} - q_n}{h}$$

$$q(t_{n+\frac{1}{2}}) \approx \frac{1}{\cos \nu} \frac{q_{n+1} + q_n}{2}$$

S/V : $q_{n+1} - 2q_n + q_{n-1} = h^2 \text{sinc}^2 \nu f_n$

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$v(t_n) \approx \dot{p}(t_n) = \frac{1}{\text{sinc } 2\nu} \frac{q_{n+1} - q_{n-1}}{2}$$



$$v(t_{n+\frac{1}{2}}) \approx \frac{1}{\text{sinc } \nu} \frac{q_{n+1} - q_n}{h}$$

$$q(t_{n+\frac{1}{2}}) \approx \frac{1}{\cos \nu} \frac{q_{n+1} + q_n}{2}$$

$$v(t_{n-\frac{1}{2}}) \approx \frac{1}{\text{sinc } \nu} \frac{q_n - q_{n-1}}{h}$$

$$q(t_{n-\frac{1}{2}}) \approx \frac{1}{\cos \nu} \frac{q_n + q_{n-1}}{2}$$

S/V_{EF}: one-step formulation

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$(1) \quad q_{n+1} - 2q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu f(q_n)$$

$$(2) \quad v_n = \frac{1}{\operatorname{sinc} 2\nu} \frac{q_{n+1} - q_{n-1}}{2h} \quad (3) \quad v_{n+\frac{1}{2}} = \frac{1}{\operatorname{sinc} \nu} \frac{q_{n+1} - q_n}{h}$$

$$(1) \text{ and } (2) : v_{n+\frac{1}{2}} = \frac{1}{\operatorname{sinc} \nu} \frac{q_{n+1} - q_n}{h} = \cos \nu v_n + \frac{h}{2} \operatorname{sinc} \nu f(q_n)$$

$$v_{n+\frac{1}{2}} = \cos \nu v_n + \frac{h}{2} \operatorname{sinc} \nu f(q_n) \quad q_{n+1} = q_n + h \operatorname{sinc} \nu v_{n+\frac{1}{2}}$$

$$q_{n+1} - 2q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu f(q_n)$$

$$+ \quad q_{n+2} - 2q_{n+1} + q_n = h^2 \operatorname{sinc}^2 \nu f(q_{n+1})$$

$$q_{n+2} - q_{n+1} - q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu (f(q_n) + f(q_{n+1}))$$

$$\iff \frac{q_{n+2} - q_n}{2h \operatorname{sinc} 2\nu} - \frac{q_{n+1} - q_{n-1}}{2h \operatorname{sinc} 2\nu} = \frac{h}{2} \operatorname{tanc} \nu (f(q_n) + f(q_{n+1}))$$

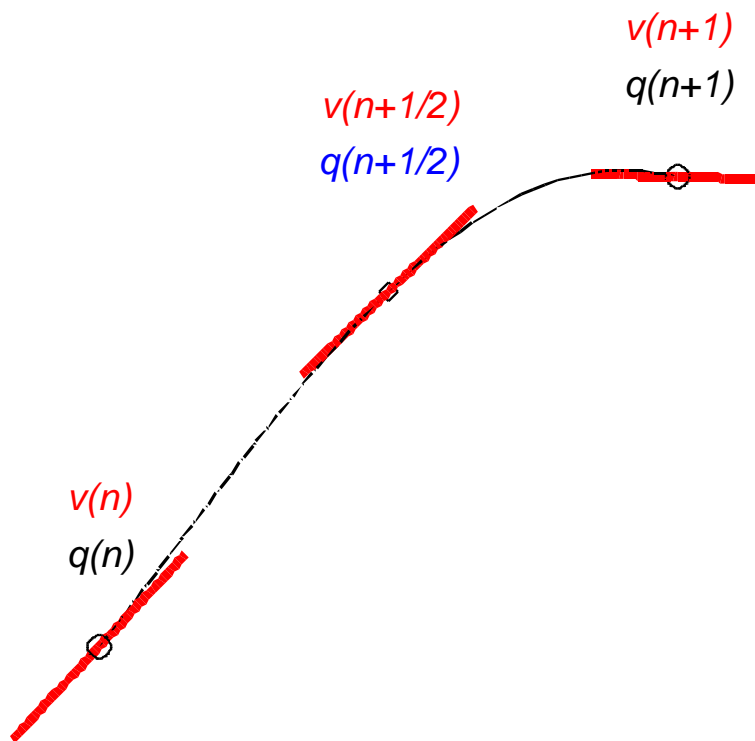
$$\iff v_{n+1} - v_n = \frac{h}{2} \operatorname{tanc} \nu (f(q_n) + f(q_{n+1}))$$

$$v_{n+1} = \frac{1}{\cos \nu} v_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{tanc} \nu f(q_{n+1})$$

S/V_{EF}: one-step formulation

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$\Phi_h^A : (q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$$



(A_{EF})

$$v_{n+\frac{1}{2}} = \cos \nu v_n + \frac{h}{2} \operatorname{sinc} \nu f(q_n)$$

EF expl. Euler, $h/2$

$$q_{n+1} = q_n + h \operatorname{sinc} \nu v_{n+\frac{1}{2}}$$

EF expl. midpoint, h

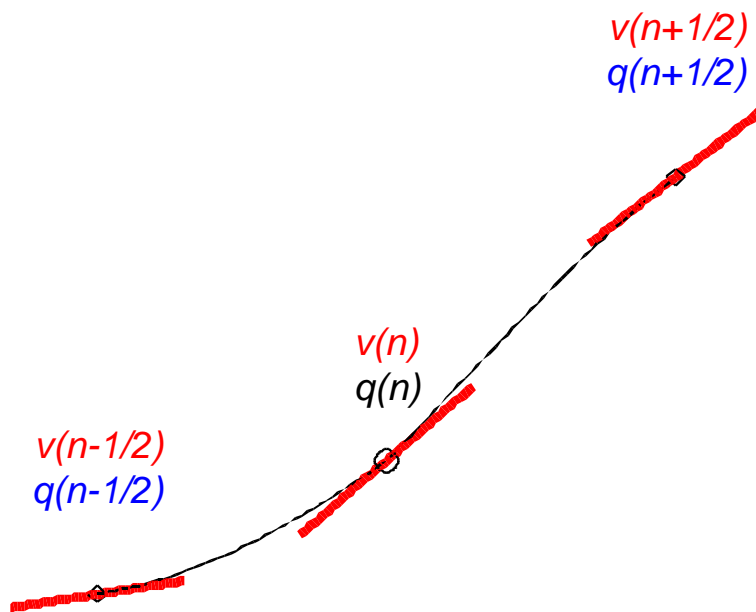
$$v_{n+1} = \frac{1}{\cos \nu} v_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{tanc} \nu f(q_{n+1})$$

EF impl. Euler, $h/2$

S/V_{EF}: one-step formulation

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$\Phi_h^B : (q_{n-\frac{1}{2}}, v_{n-\frac{1}{2}}) \mapsto (q_{n+\frac{1}{2}}, v_{n+\frac{1}{2}})$$



(B_{EF})

$$q_n = \cos \nu q_{n-\frac{1}{2}} + \frac{h}{2} \operatorname{sinc} \nu v_{n-\frac{1}{2}}$$

EF expl. Euler, $h/2$

$$v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + h \operatorname{sinc} \nu f(q_n)$$

EF expl. midpoint, h

$$q_{n+\frac{1}{2}} = \frac{1}{\cos \nu} q_n + \frac{h}{2} \operatorname{tanc} \nu v_{n+\frac{1}{2}}$$

EF impl. Euler, $h/2$

S/V_{EF}: one-step formulation

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$(A_{EF}) : \begin{cases} v_{n+\frac{1}{2}} = \cos \nu v_n + \frac{h}{2} \operatorname{sinc} \nu f(q_n) \\ q_{n+1} = q_n + h \operatorname{sinc} \nu v_{n+\frac{1}{2}} \\ v_{n+1} = \frac{1}{\cos \nu} v_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{tanc} \nu f(q_{n+1}) \end{cases}$$

$$\begin{cases} q_{n+1} = q_n + h \operatorname{sinc} \nu v_{n+\frac{1}{2}} \\ v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + h \operatorname{sinc} \nu f(q_n) \end{cases}$$

$$(B_{EF}) : \begin{cases} q_n = \cos \nu q_{n-\frac{1}{2}} + \frac{h}{2} \operatorname{sinc} \nu v_{n-\frac{1}{2}} \\ v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + h \operatorname{sinc} \nu f(q_n) \\ q_{n+\frac{1}{2}} = \frac{1}{\cos \nu} q_n + \frac{h}{2} \operatorname{tanc} \nu v_{n+\frac{1}{2}} \end{cases}$$

The Störmer-Verlet method

- construction
- one-step formulation
- composition method

S/V_{EF}: composition method

$$\dot{q} = v \quad \dot{v} = f(q)$$

$$(A_{EF}) : \begin{cases} v_{n+\frac{1}{2}} = \cos \nu v_n + \frac{h}{2} \operatorname{sinc} \nu f(q_n) \\ q_{n+1} = q_n + h \operatorname{sinc} \nu v_{n+\frac{1}{2}} \\ v_{n+1} = \frac{1}{\cos \nu} v_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{tanc} \nu f(q_{n+1}) \end{cases} \begin{cases} q_{n+\frac{1}{2}} = \frac{1}{\cos \nu} q_n + \frac{h}{2} \operatorname{tanc} \nu v_{n+\frac{1}{2}} \\ q_{n+1} = \cos \nu q_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{sinc} \nu v_{n+\frac{1}{2}} \end{cases}$$

$$(SE1_{EF}) \begin{cases} v_{n+\frac{1}{2}} = \cos \nu v_n + \frac{h}{2} \operatorname{sinc} \nu f(q_n) \\ q_{n+\frac{1}{2}} = \frac{1}{\cos \nu} q_n + \frac{h}{2} \operatorname{tanc} \nu v_{n+\frac{1}{2}} \end{cases}$$

$$(SE2_{EF}) \begin{cases} q_{n+1} = \cos \nu q_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{sinc} \nu v_{n+\frac{1}{2}} \\ v_{n+1} = \frac{1}{\cos \nu} v_{n+\frac{1}{2}} + \frac{h}{2} \operatorname{tanc} \nu f(q_{n+1}) \end{cases}$$

$$(A_{EF}) = (SE2_{EF}) \circ (SE1_{EF})$$

$$(B_{EF}) = (SE1_{EF}) \circ (SE2_{EF})$$

The Störmer-Verlet method

- construction
- one-step formulation
- composition method
- splitting method

S/V_{EF}: splitting method

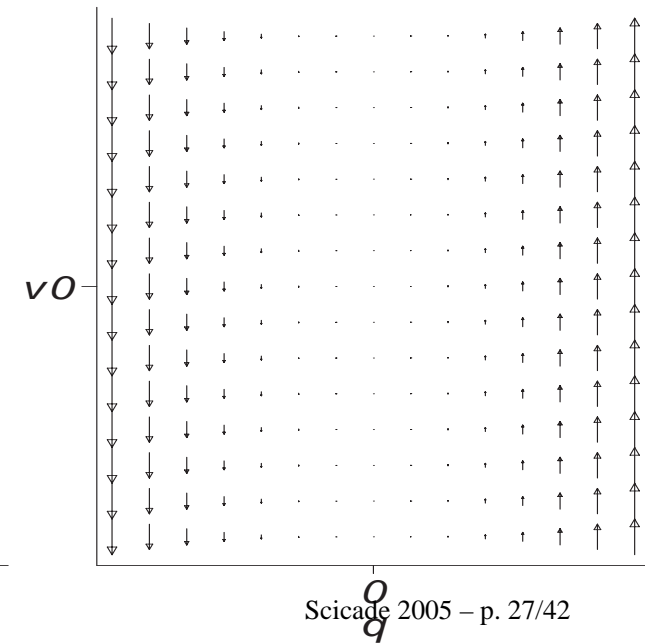
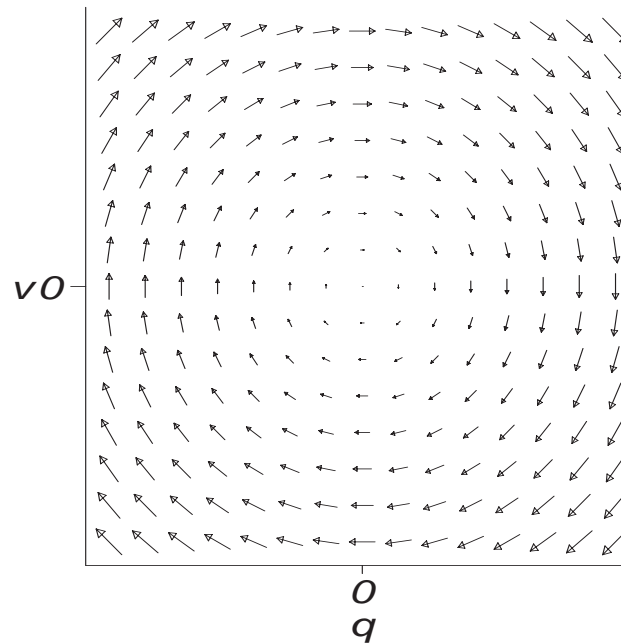
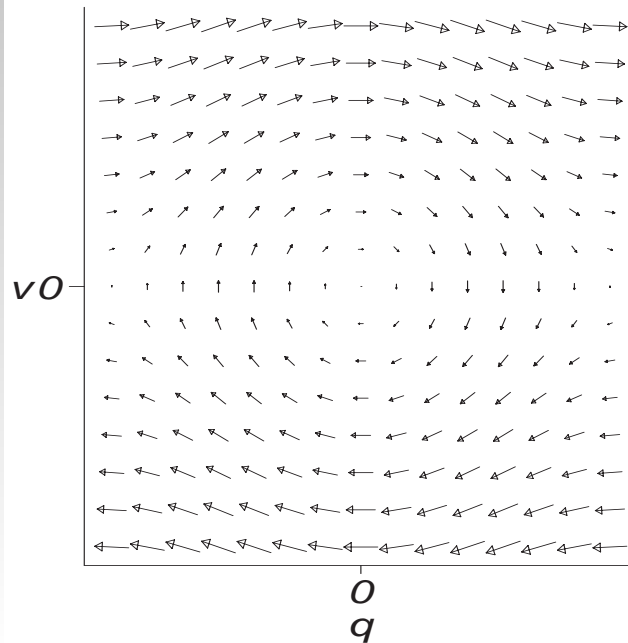
$$\ddot{q} = f(q) = g(q) - \omega^2 q \iff \ddot{q} + \omega^2 q = g(q) \iff \begin{cases} \dot{q} = v \\ \dot{v} = g(q) - \omega^2 q \end{cases}$$

Split the vector field

$$(v, g(q) - \omega^2 q) = (v, -\omega^2 q) + (0, g(q))$$

Example : $\ddot{q} = -\sin q$

$$(v, -\sin q) = (v, -q) + (0, q - \sin q)$$



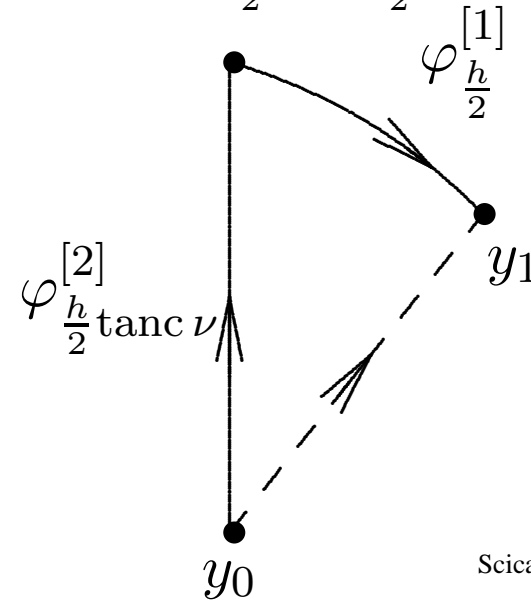
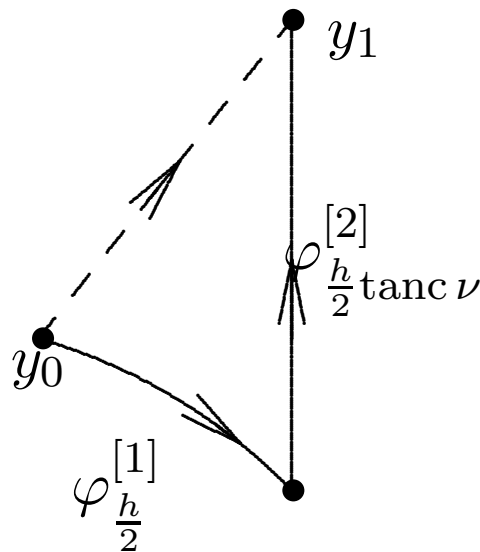
S/V_{EF}: splitting method

$$\begin{aligned} \dot{q} = v \quad \dot{v} = g(q) - \omega^2 q = f(q) \\ (v, g(q) - \omega^2 q) = (v, -\omega^2 q) + (0, g(q)) \end{aligned}$$

The exact flows $\varphi_t^{[1]}$ and $\varphi_t^{[2]}$ of these two vector fields are

$$\varphi_t^{[1]} : \begin{cases} q_1 = q_0 \cos \omega t + \frac{v_0}{\omega} \sin \omega t \\ v_1 = -\omega q_0 \sin \omega t + v_0 \cos \omega t \end{cases} \quad \varphi_t^{[2]} : \begin{cases} q_1 = q_0 \\ v_1 = v_0 + t g(q_0) \end{cases}$$

$$(\text{SE2}_{\text{EF}}) = \varphi_{\frac{h}{2} \text{tanc } \nu}^{[2]} \circ \varphi_{\frac{h}{2}}^{[1]} \quad (\text{SE1}_{\text{EF}}) = \varphi_{\frac{h}{2}}^{[1]} \circ \varphi_{\frac{h}{2} \text{tanc } \nu}^{[2]}$$

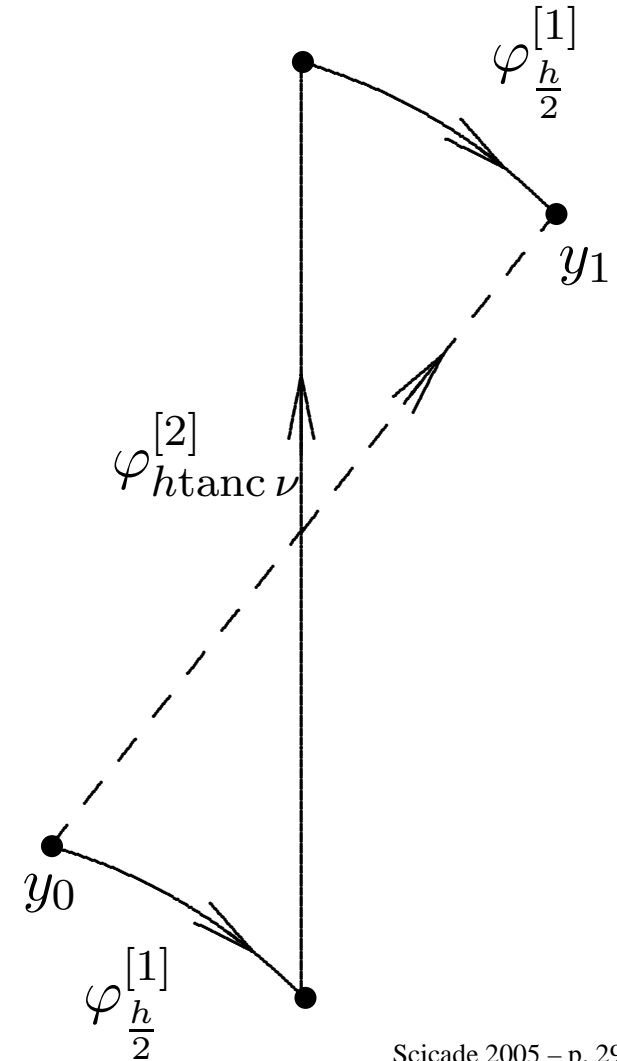
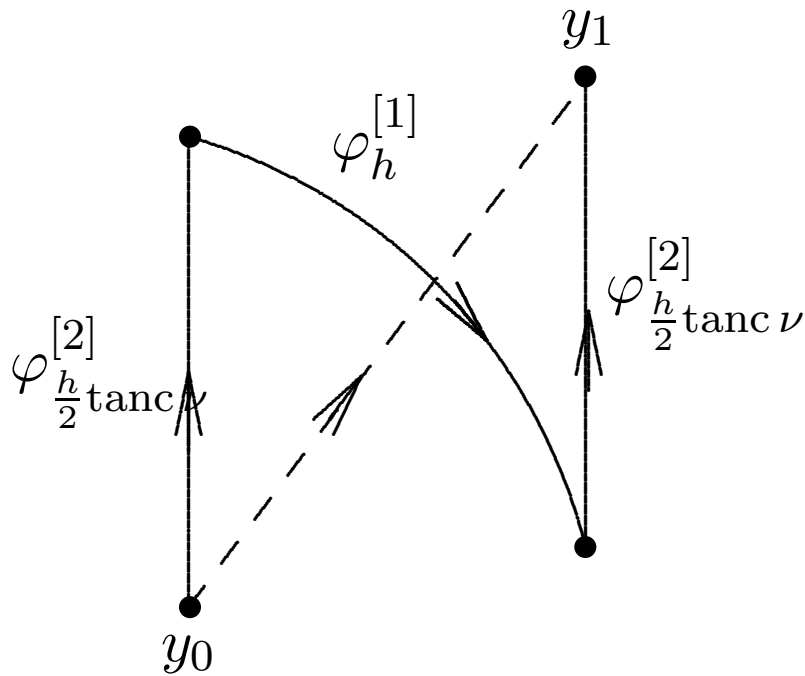


S/V_{EF}: splitting method

$$\dot{q} = v \quad \dot{v} = g(q) - \omega^2 q = f(q)$$

$$(A_{EF}) = (SE2_{EF}) \circ (SE1_{EF})$$

$$(B_{EF}) = (SE1_{EF}) \circ (SE2_{EF})$$



The Störmer-Verlet method

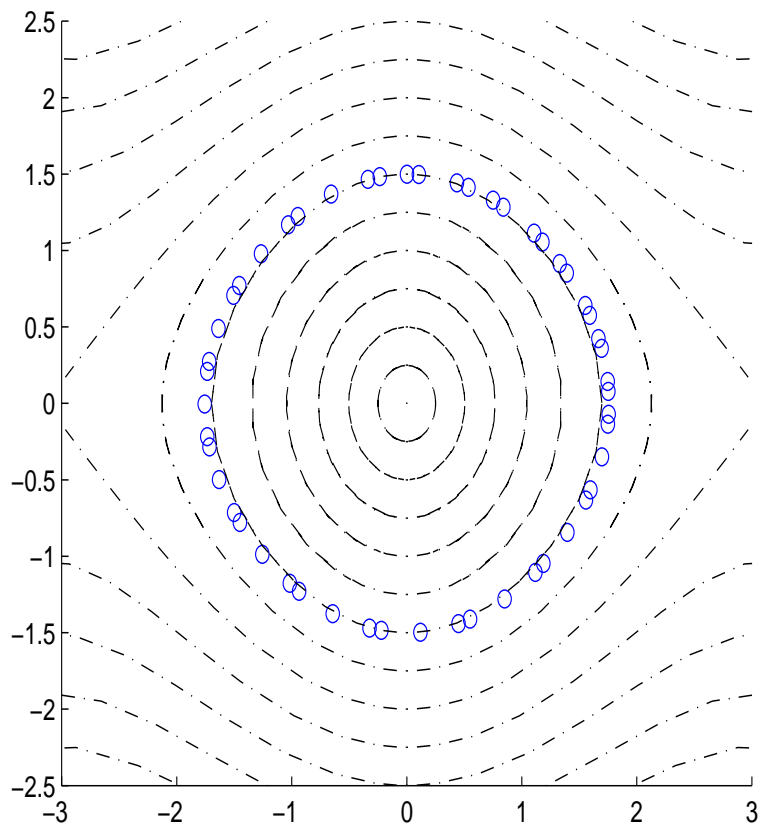
- construction
- one-step formulation
- composition method
- splitting method
- variational integrator

The pendulum

$$\ddot{q} = -\sin q, \quad q(0) = 0, \quad \dot{q}(0) = 1.5$$

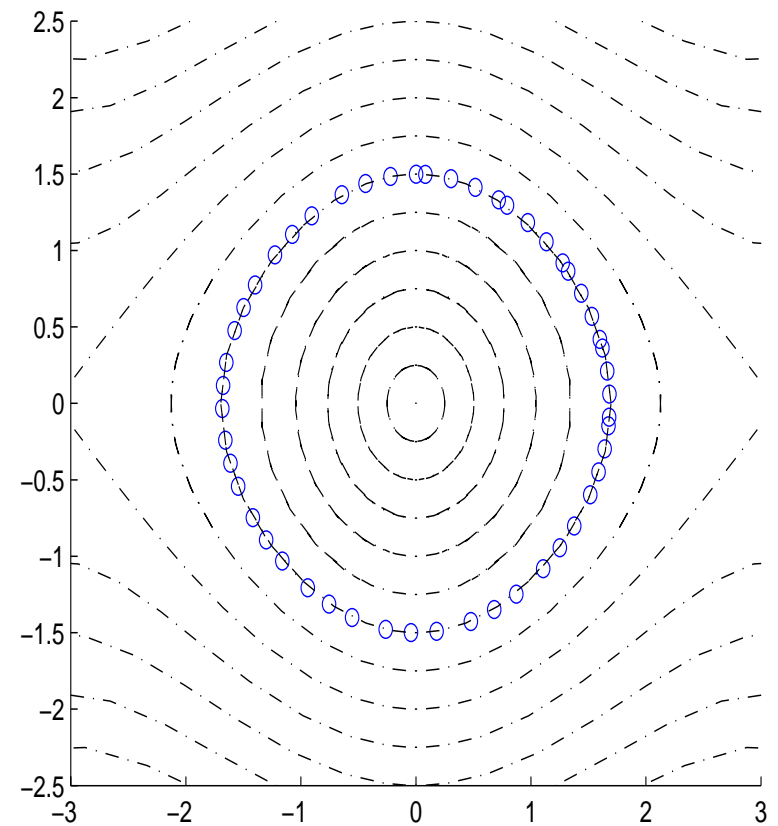
$$h = 0.5, 50 \text{ steps}$$

(A)



(A_{EF})

$$\omega = 1$$

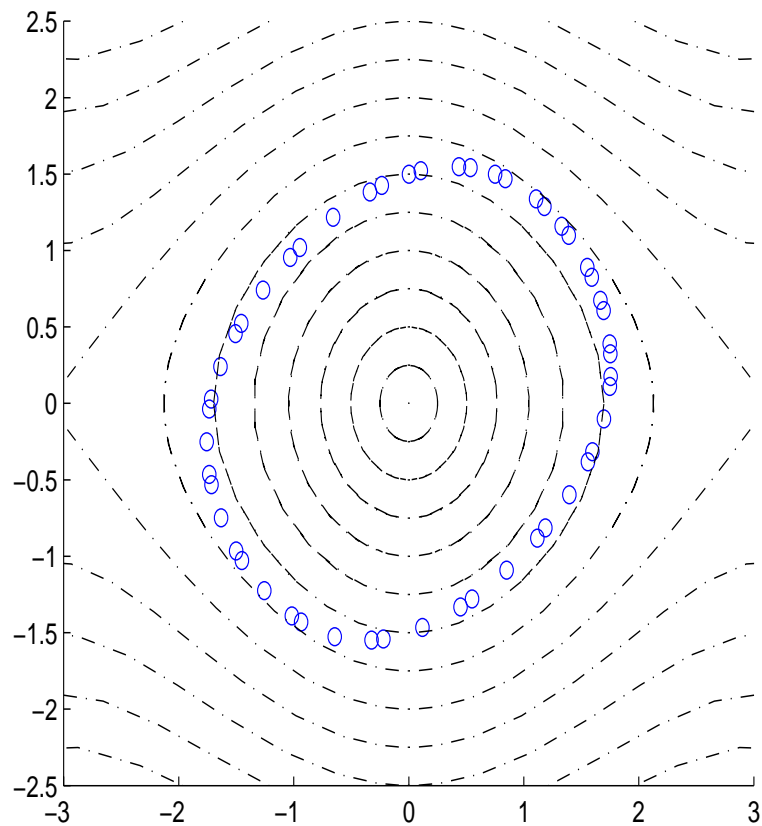


The pendulum

$$\ddot{q} = -\sin q, \quad q(0) = 0, \quad \dot{q}(0) = 1.5$$

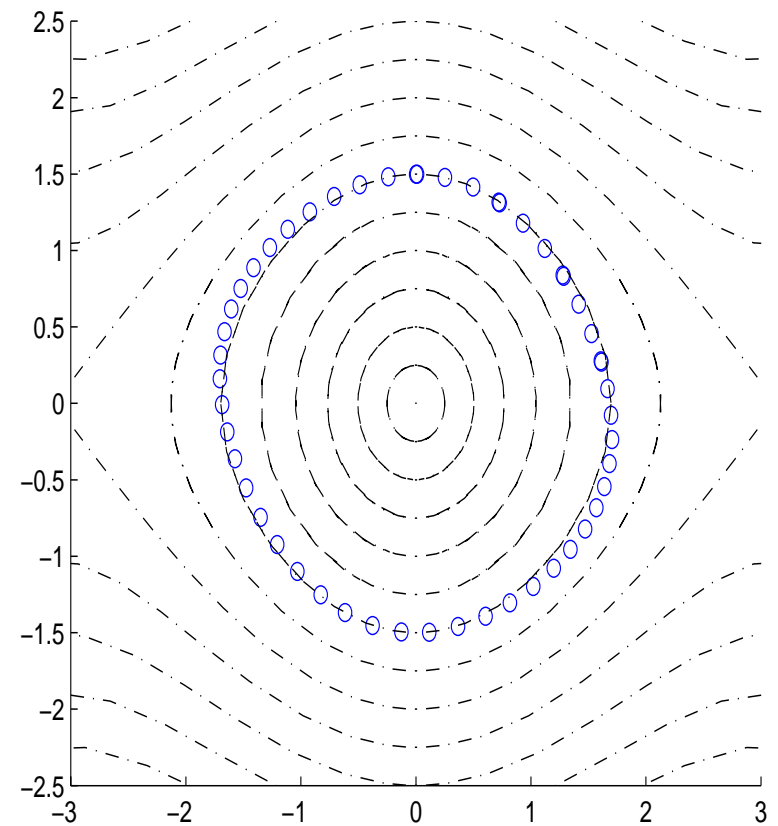
$$h = 0.5, 50 \text{ steps}$$

SE1



SE1_{EF}

$$\omega = 1$$



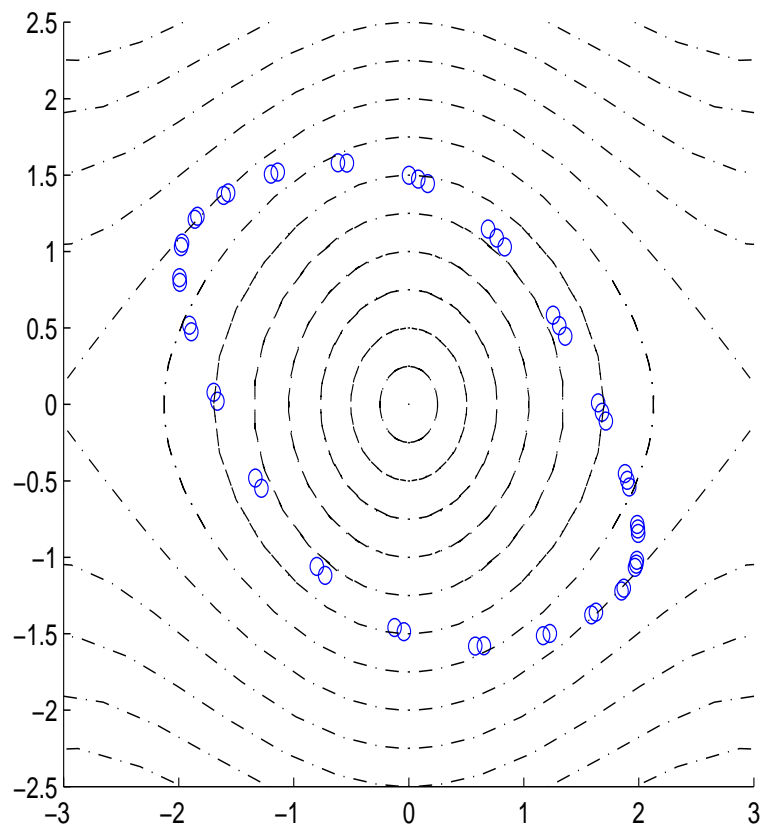
The pendulum

$$\ddot{q} = -\sin q, \quad q(0) = 0, \quad \dot{q}(0) = 1.5$$

$$h = 0.5, 50 \text{ steps}$$

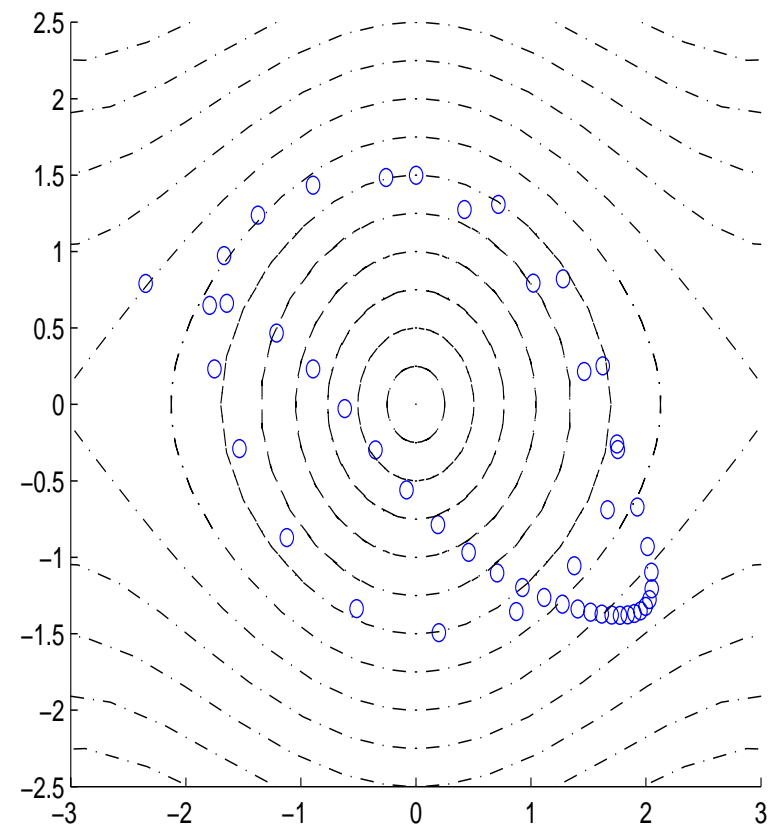
SE1_{EF}

$$\omega = 1.4$$



SE1_{EF}

$$\omega_n = 1 + n/50$$



The Störmer-Verlet method

- construction
- one-step formulation
- composition method
- splitting method
- variational integrator

Example : ω must be held constant

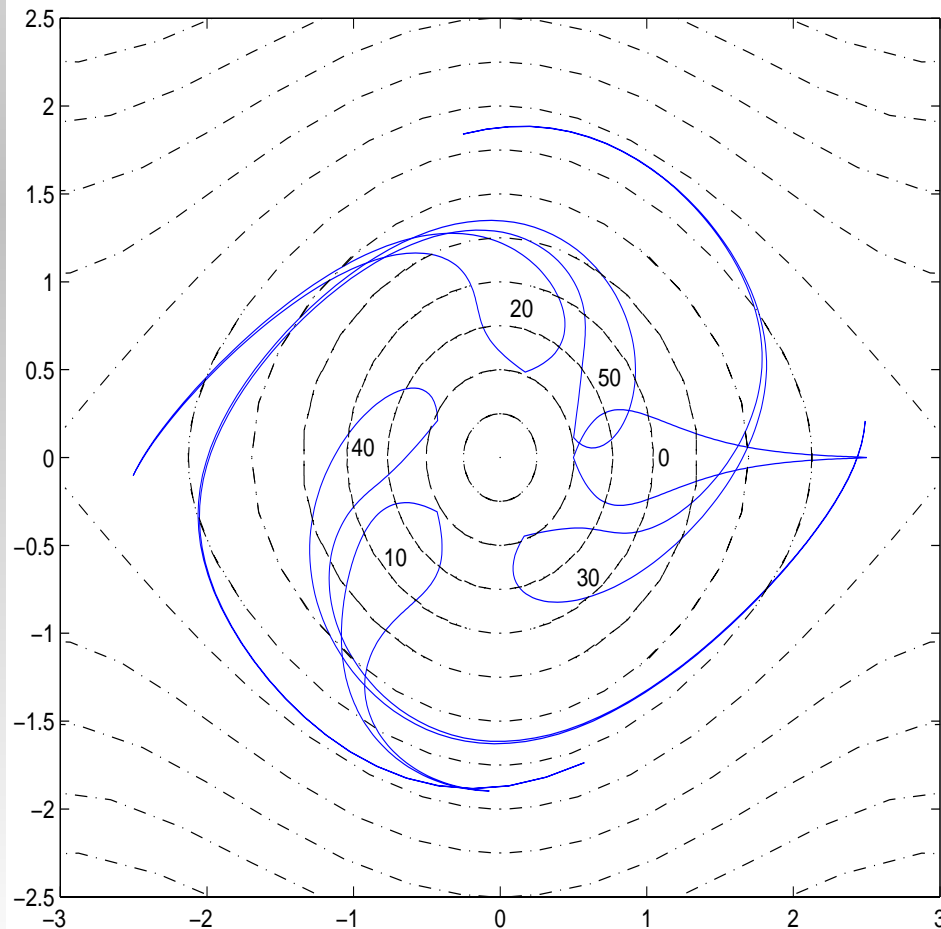
- geometric properties
 - symmetry and reversibility
 - symplecticity

The pendulum : symplecticity

$$\ddot{q} = -\sin q$$

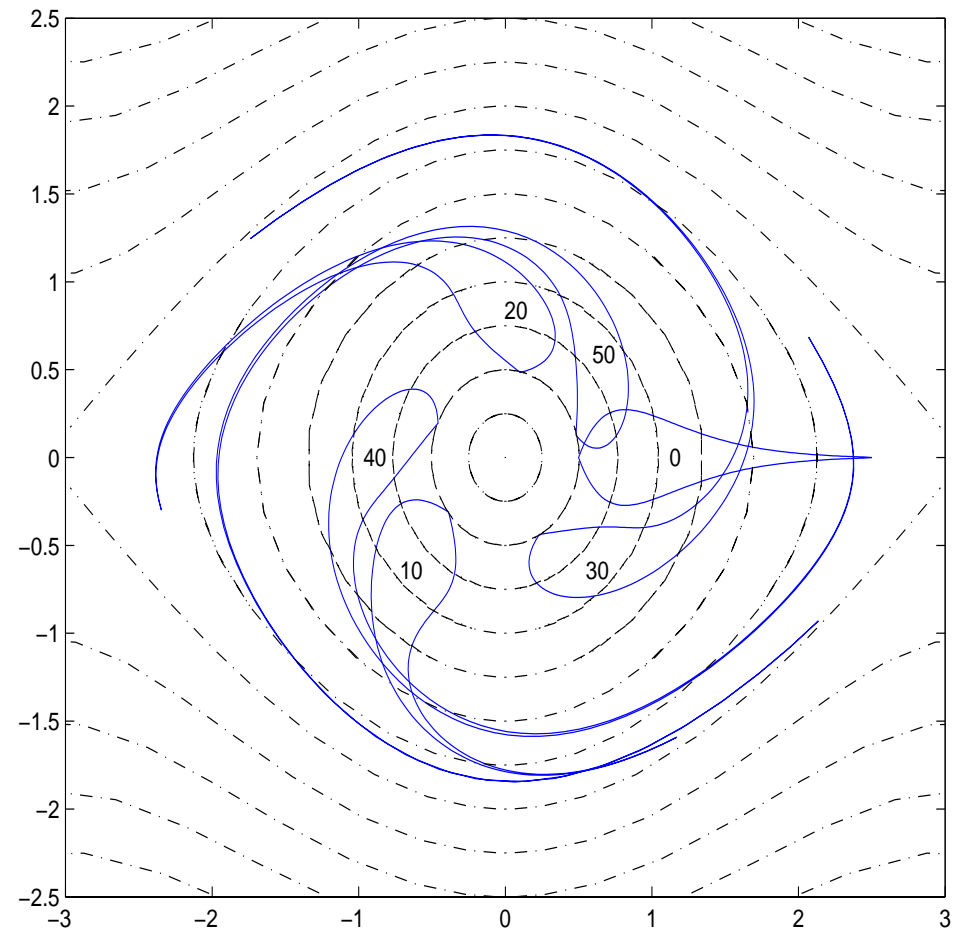
$$h = 0.25, 50 \text{ steps}$$

SE1



SE1_{EF}

$$\omega = 1$$

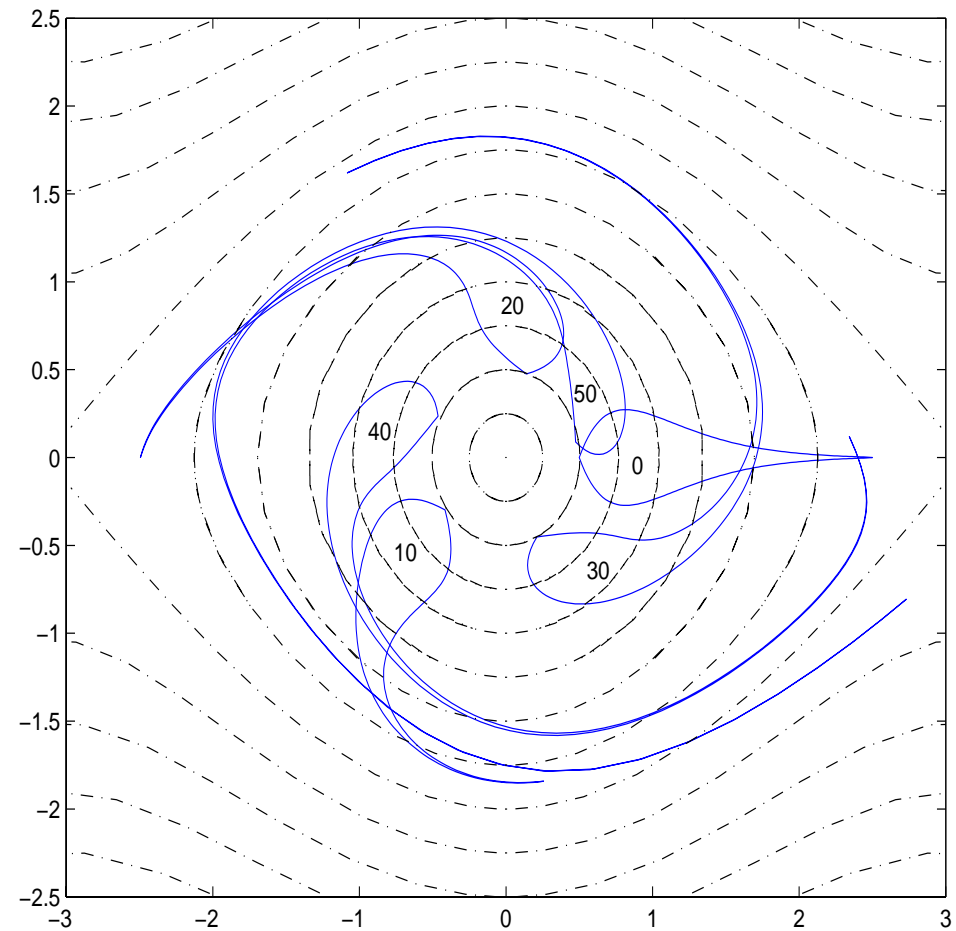


The pendulum : symplecticity

$$\ddot{q} = -\sin q$$

$$h = 0.25, 50 \text{ steps}$$

$$\text{SE1}_{\text{EF}} \quad \omega_n = 1 + n/50$$



Conclusion

The exponential fitted versions
of the SE and the S/V

- give **periodic** solutions are obtained as long as ω is **fixed**.
- are symplectic, even if ω varies from step to step.

Problem

How to obtain a good fixed choice for ω ?

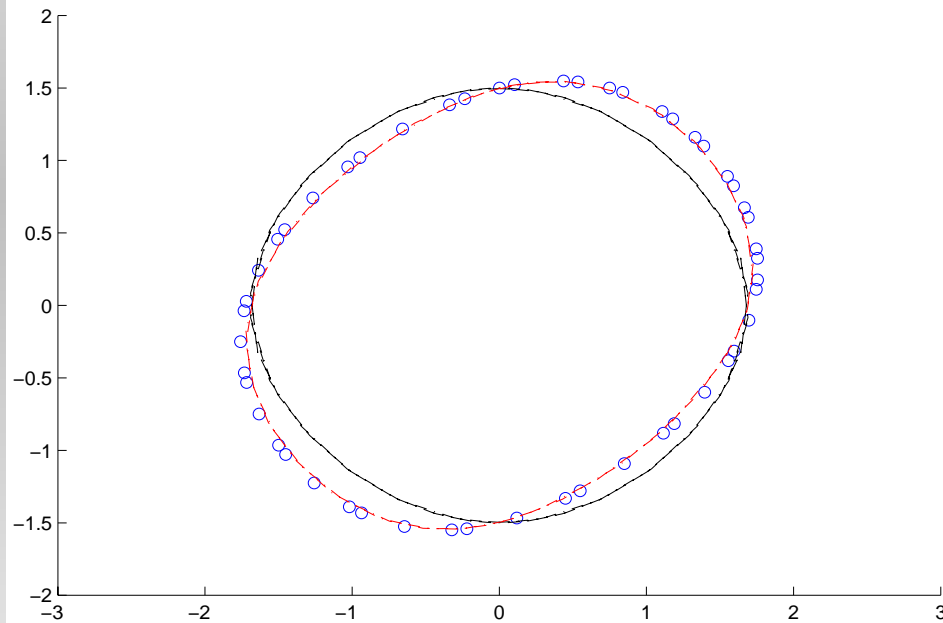
- study of modified equation : backward error analysis
- study of error in H

The pendulum : modified eqn.

$$\ddot{q} = -\sin q, \quad q(0) = 0, \quad \dot{q}(0) = 1.5$$

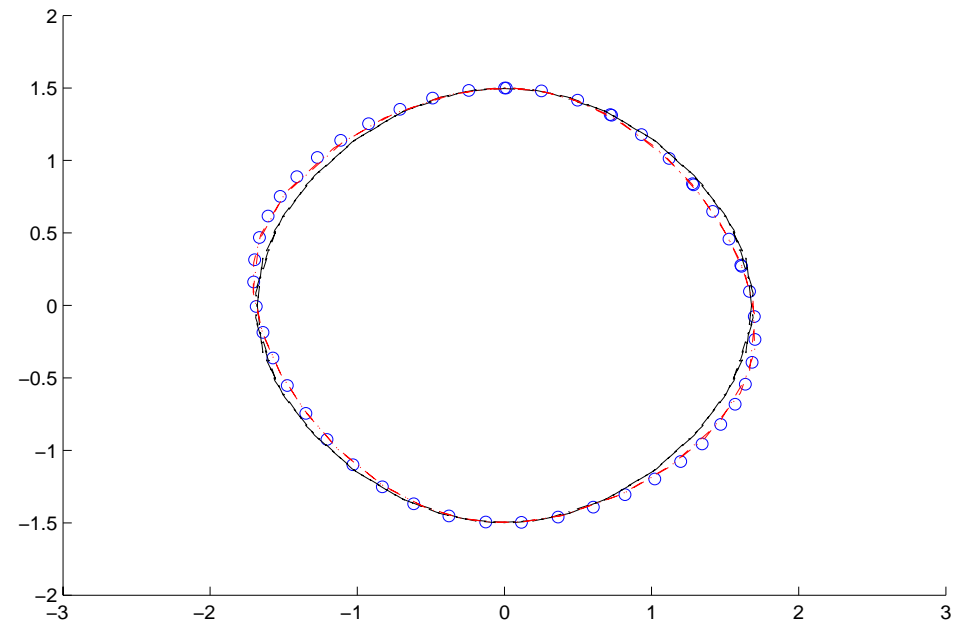
$$h = 0.25, 50 \text{ steps}$$

SE1



SE1_{EF}

$$\omega = 1$$



$$\dot{q} = v + \frac{h}{2} (\omega^2 q - \sin(q)) + \mathcal{O}(h^2)$$

$$\dot{v} = -\sin q + \frac{h}{2} (\cos q - \omega^2) + \mathcal{O}(h^2)$$

The pendulum : error in H

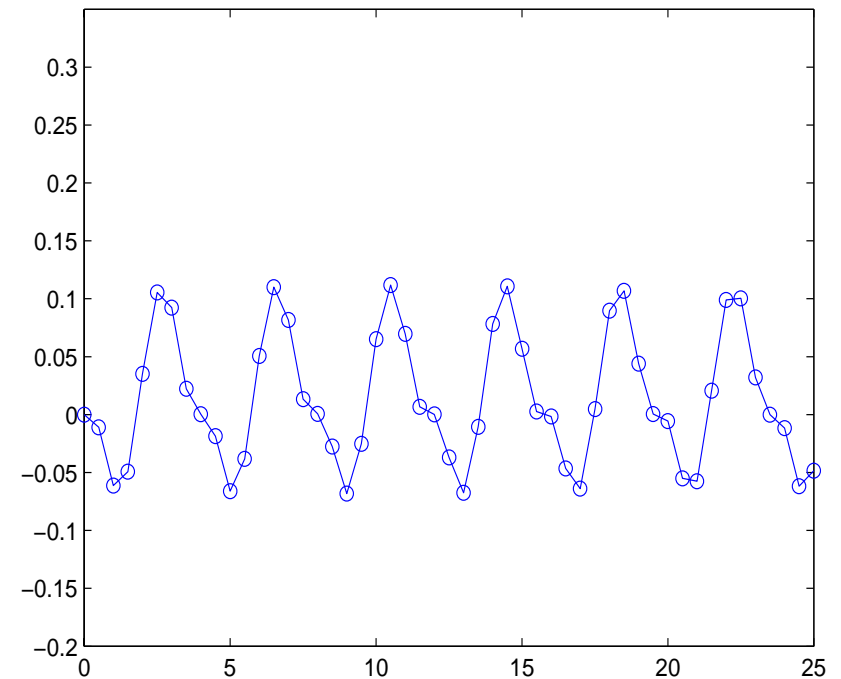
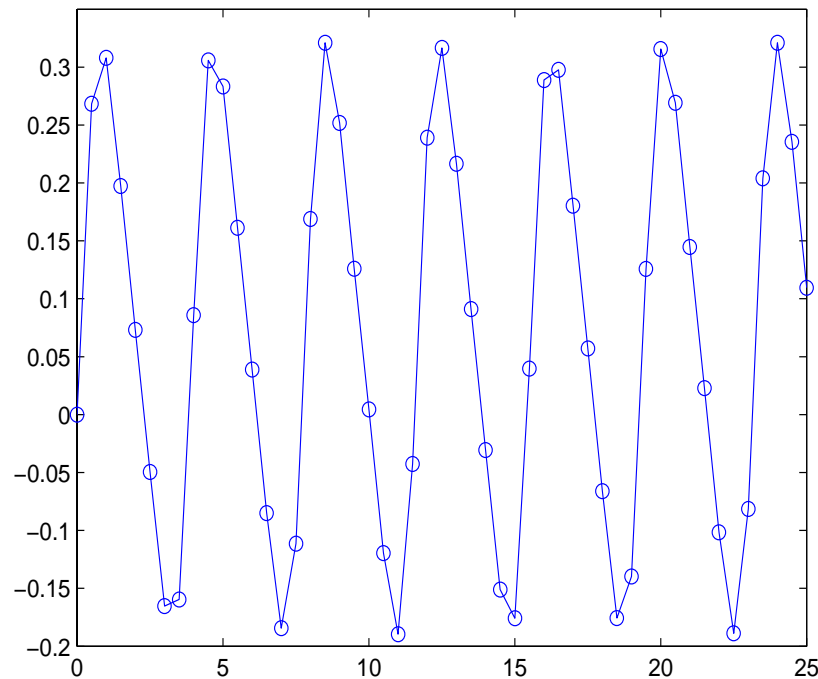
$$\ddot{q} = -\sin q, \quad q(0) = 0, \quad \dot{q}(0) = 1.5$$

$$h = 0.5, \text{ 50 steps}$$

SE1

SE1_{EF}

$$\omega = 1$$



$$H_{n+1} = H_n + \left(\frac{1}{2} \sin q_n (\omega^2 q_n - \sin q_n) + \frac{1}{2} p_n^2 (\cos q_n - \omega^2) \right) h^2 + \mathcal{O}(h^3)$$

The pendulum : error in H

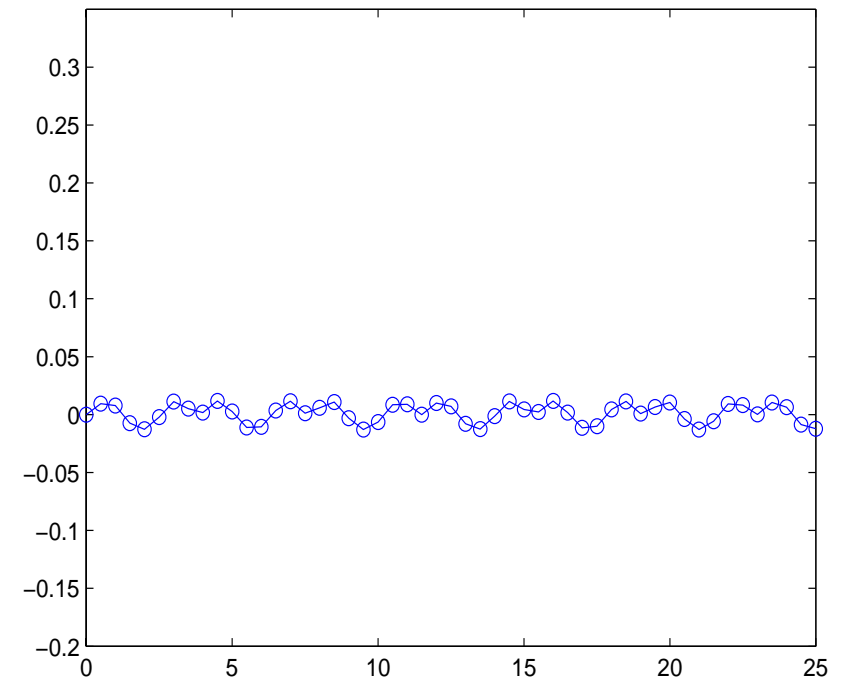
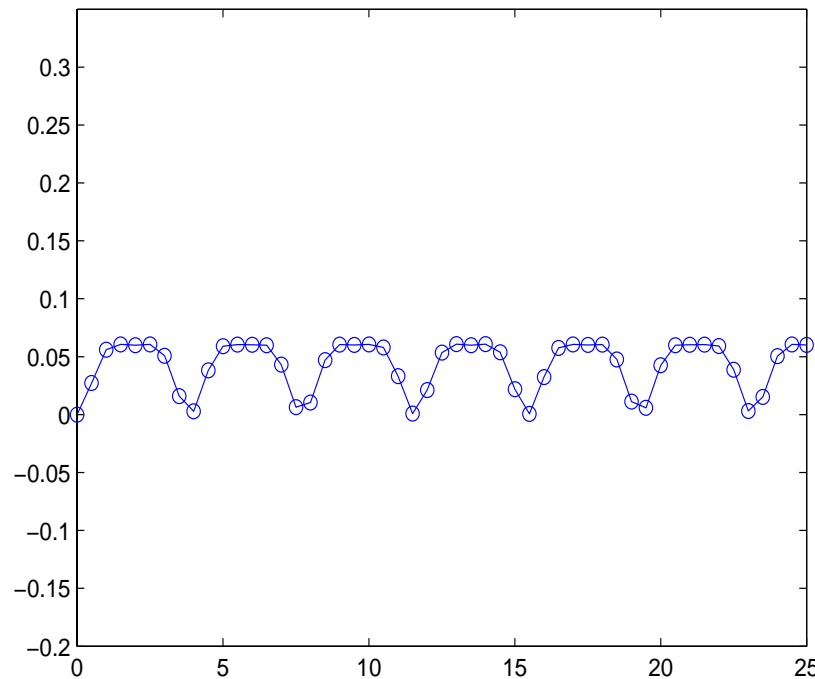
$$\ddot{q} = -\sin q, \quad q(0) = 0, \quad \dot{q}(0) = 1.5$$

$$h = 0.5, 50 \text{ steps}$$

(A)

(A_{EF})

$$\omega = 1$$



$$H_{n+1} = H_n + \frac{1}{12} \sin q_n p_n \left(3 (\omega^2 - \cos q_n) - p_n^2 \right) h^3 + \mathcal{O}(h^4)$$

Conclusion

The exponential fitted versions of the SE and the S/V with **fixed** ω have the same properties as their classical counterparts.

Fixing ω means global optimization.