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 of trigonometric behaviour.

Linear multistep methods

Well known methods to solve

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

are

- Störmer-Verlet method (order 2)

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

- Numerov method (order 4)

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

Construction

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

- Störmer-Verlet

  Replace $\ddot{q}(t) = f(q(t))$ by the interpolating polynomial
  $p(t) = a_0 + a_1\,t$ at $t_n,\ t_{n+1}$:

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

- Numerov

  Replace $\ddot{q}(t) = f(q(t))$ by the interpolating polynomial
  $p(t) = a_0 + a_1\,t + a_2\,t^2$ at $t_{n-1},\ t_n,\ t_{n+1}$:

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

Exponential fitting

Consider the initial value problem

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

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).

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

Störmer-Verlet method

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

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

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

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

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

Störmer-Verlet method

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

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

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

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

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

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

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

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

Störmer-Verlet method

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

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

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

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

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

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

$$\mathrm{sinc}\,x = \begin{cases} \dfrac{\sin x}{x} & x \neq 0 \\ 1 & x = 0 \end{cases} \qquad\qquad \mathrm{tanc}\,x = \begin{cases} \dfrac{\tan x}{x} & x \neq 0 \\ 1 & x = 0 \end{cases}$$

Numerov method

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

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

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

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

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

$\omega\,h$

Numerov method

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

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

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

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

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

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

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

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

Choice of ω

based on local truncation error

- Störmer-Verlet

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

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

- Numerov

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

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

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

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

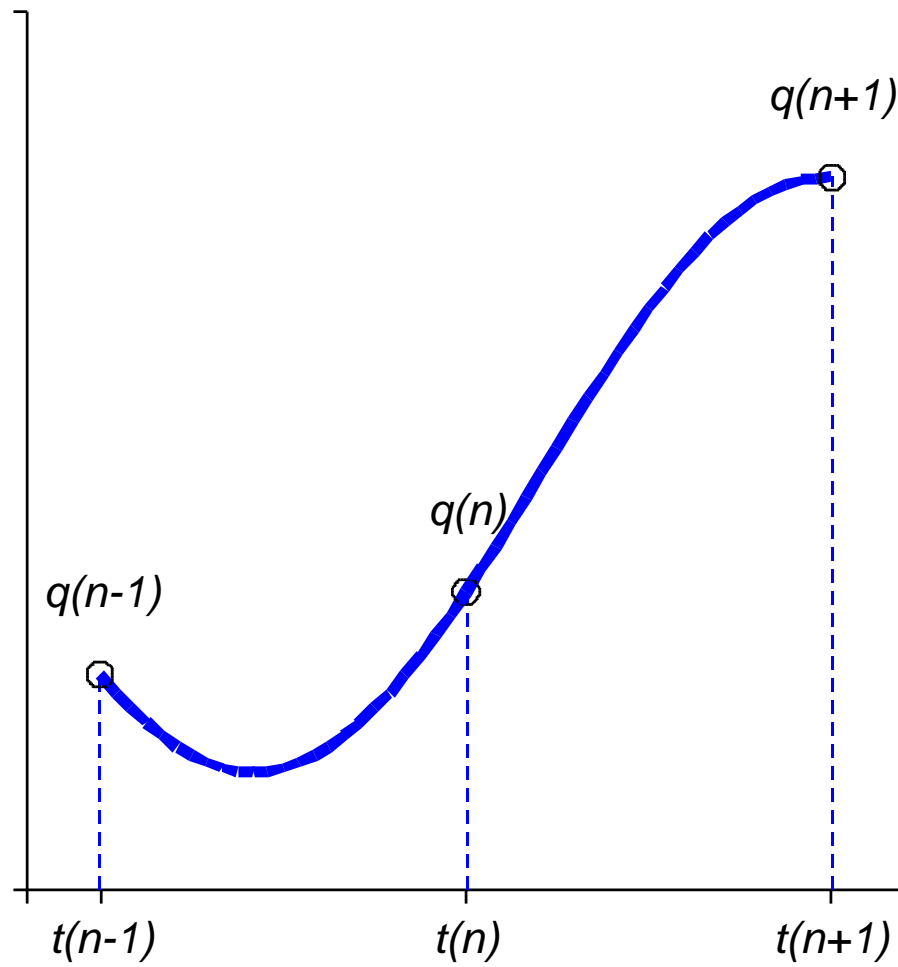Approximate $\ddot{q}(t_n) = f(q(t_n))$ by $\ddot{p}(t_n) = \dfrac{q_{n+1} - 2\, q_n + q_{n-1}}{h^2}$
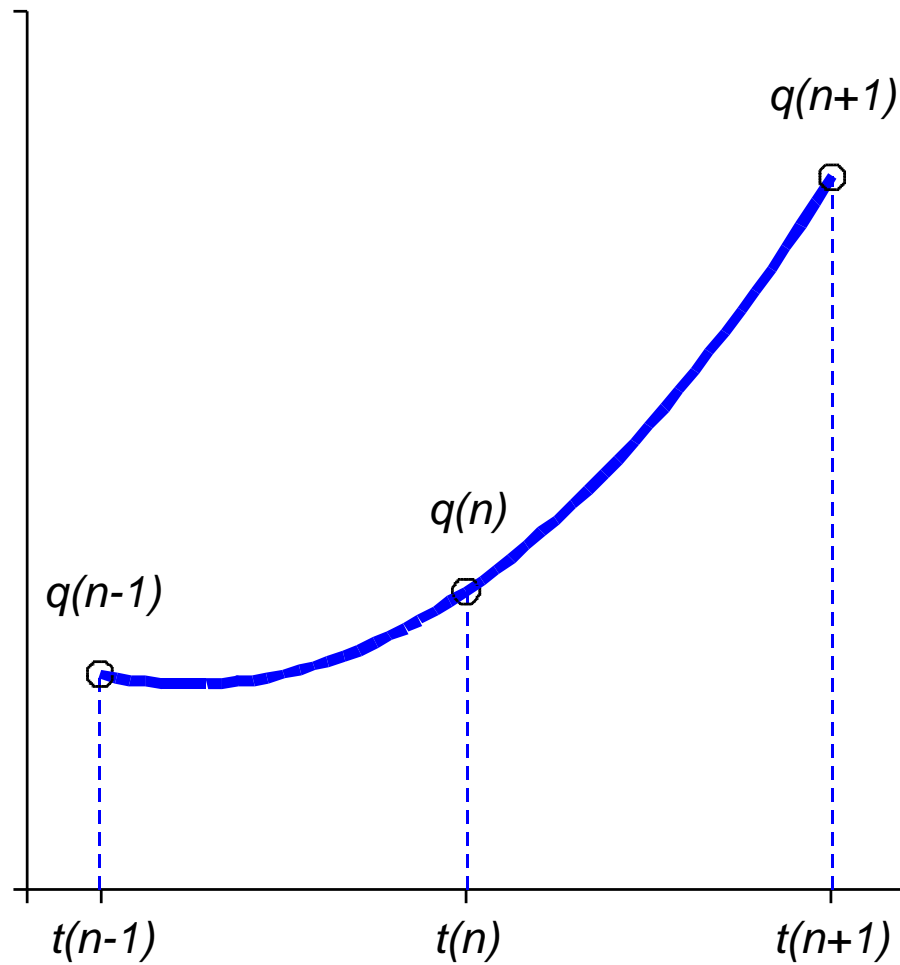
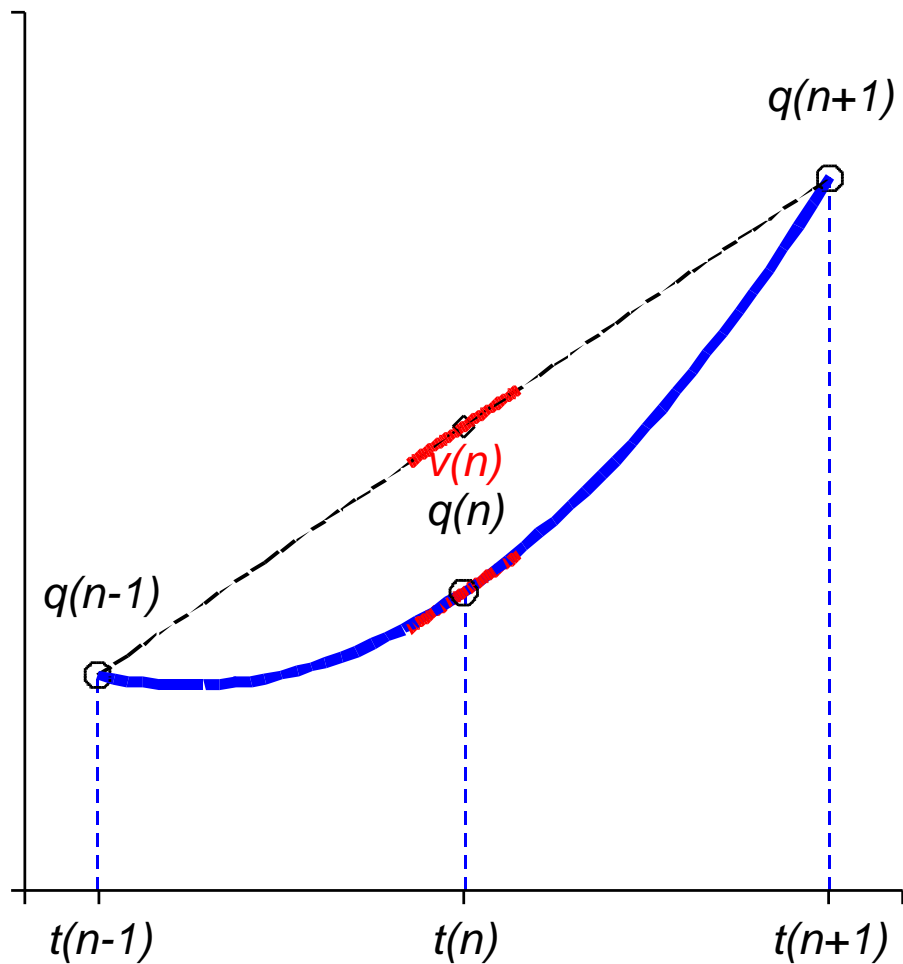# S/V$_{\textbf{EF}}$: $\quad q_{n+1} - 2\,q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu\, f_n$

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 $\ddot{p}(t_n) = \dfrac{q_{n+1} - 2\,q_n + q_{n-1}}{h^2 \operatorname{sinc}^2 \nu}$

The Störmer-Verlet method

- construction

- one-step formulation

S/V : $q_{n+1} - 2\,q_n + q_{n-1} = h^2\,f_n$
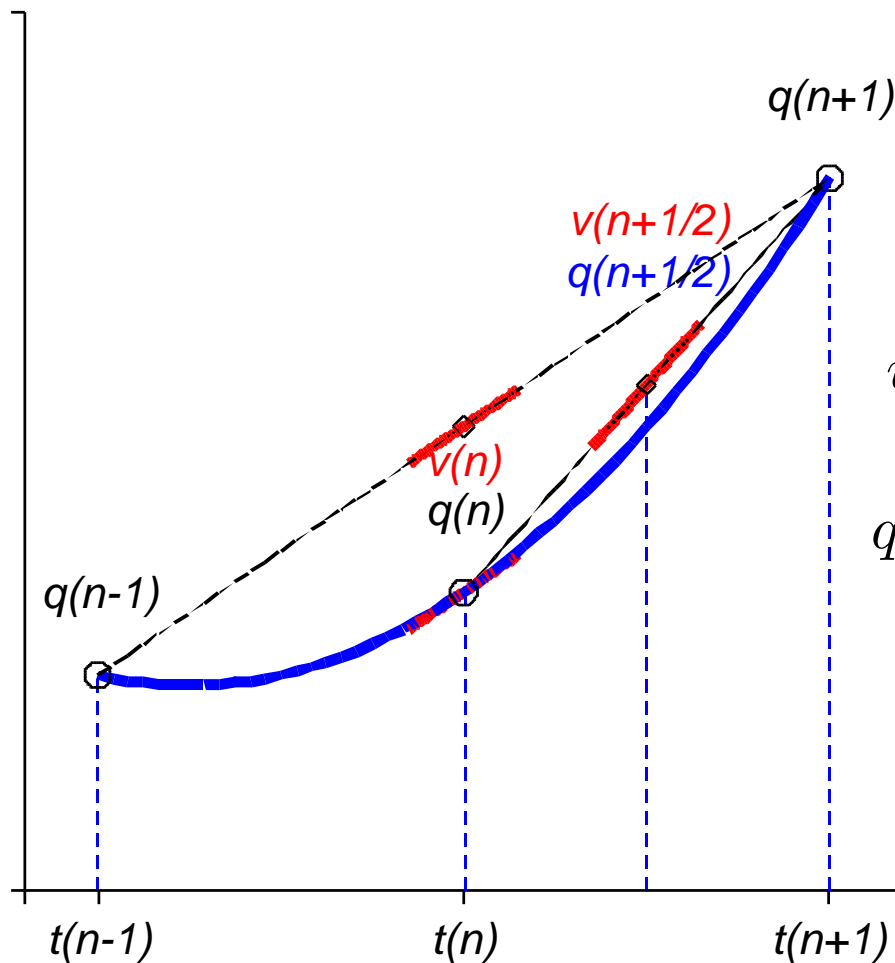
$$\dot{q} = v \qquad \dot{v} = f(q)$$

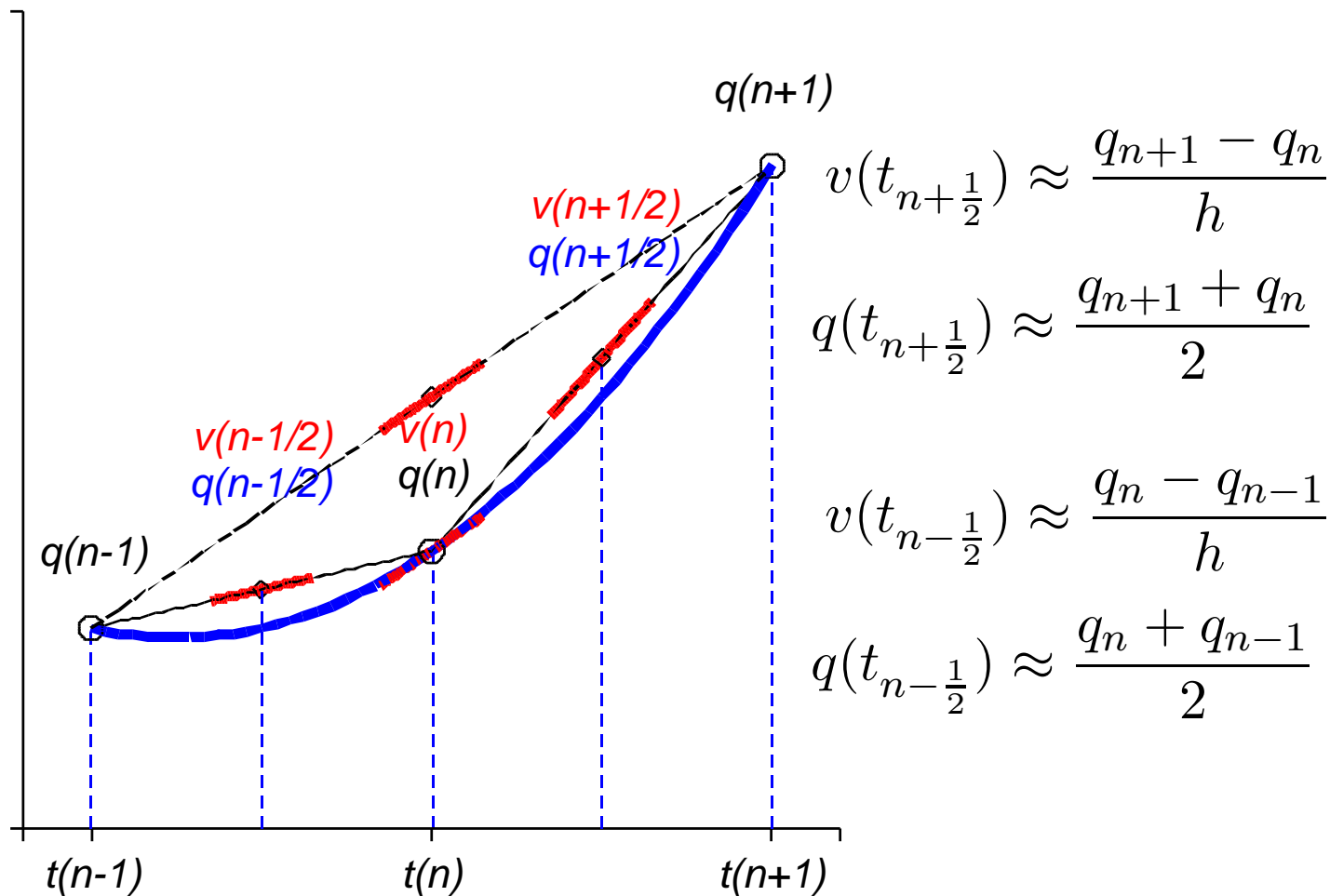$$v(t_n) \approx \dot{p}(t_n) = \frac{q_{n+1} - q_{n-1}}{2\,h}$$

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

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

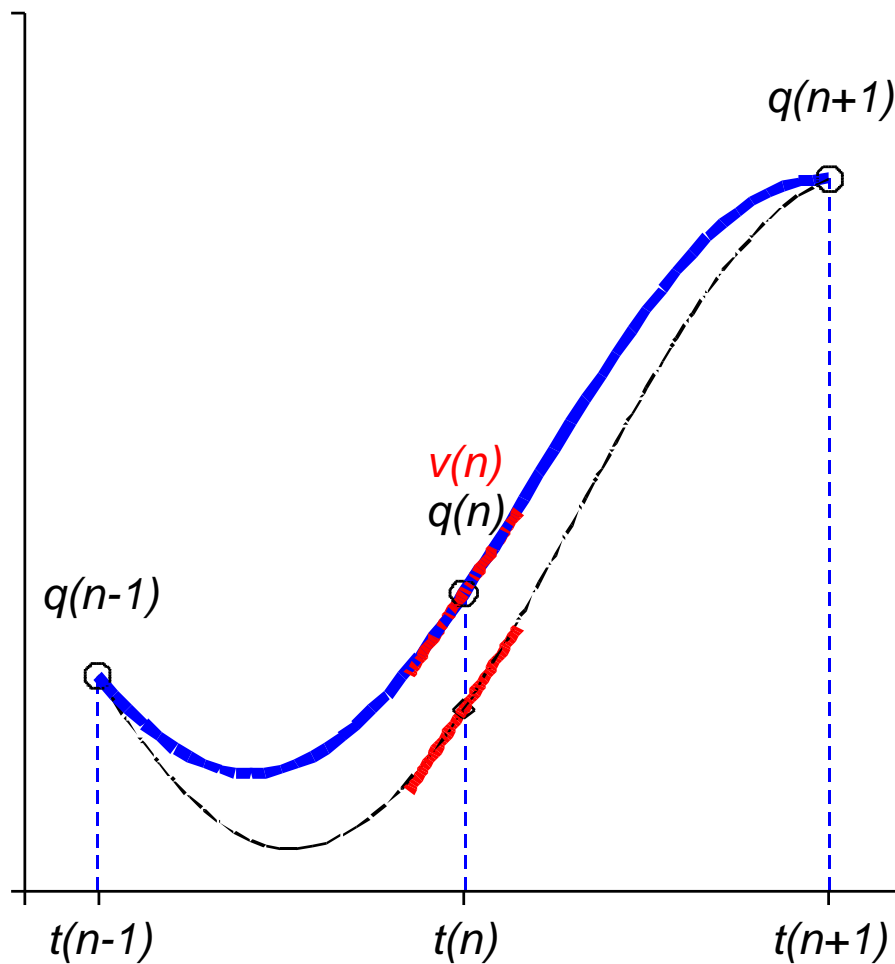$$v(t_n) \approx \dot{p}(t_n) = \frac{q_{n+1} - q_{n-1}}{2\,h}$$

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

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

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

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

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

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

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

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

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

S/V$_{\textbf{EF}}$: $\qquad q_{n+1} - 2\,q_n + q_{n-1} = h^2 \operatorname{sinc}^2 \nu\, f_n$
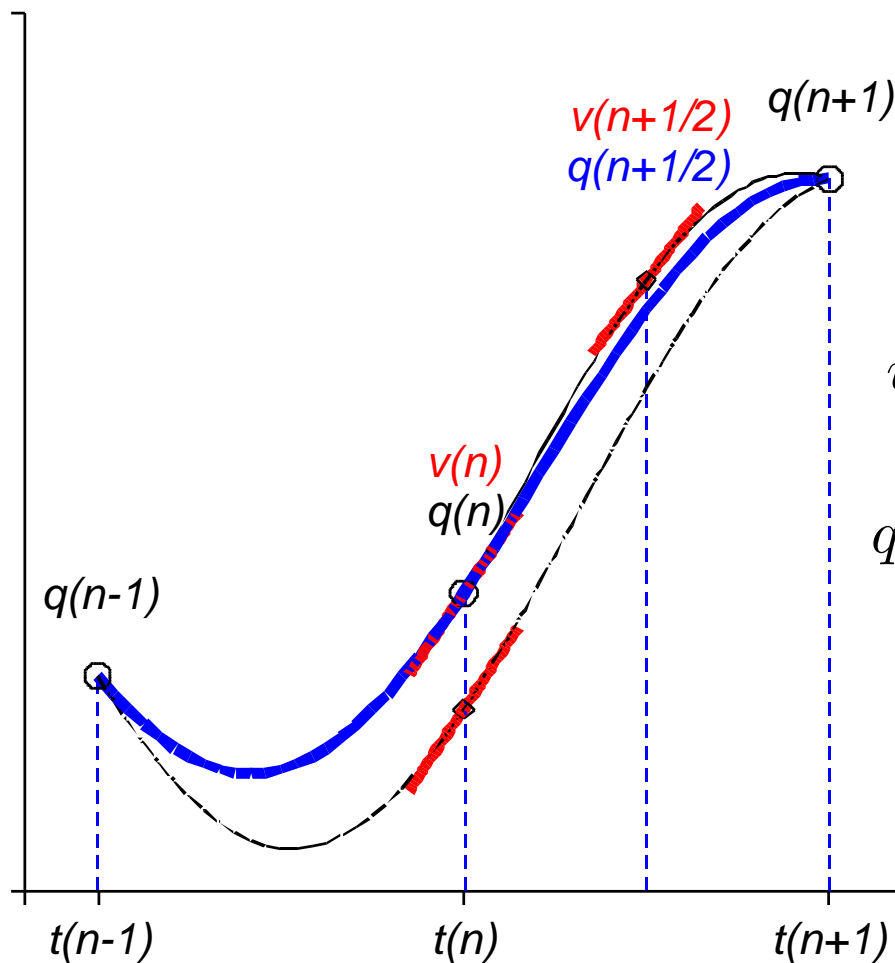
$$\dot{q} = v \qquad \dot{v} = f(q)$$

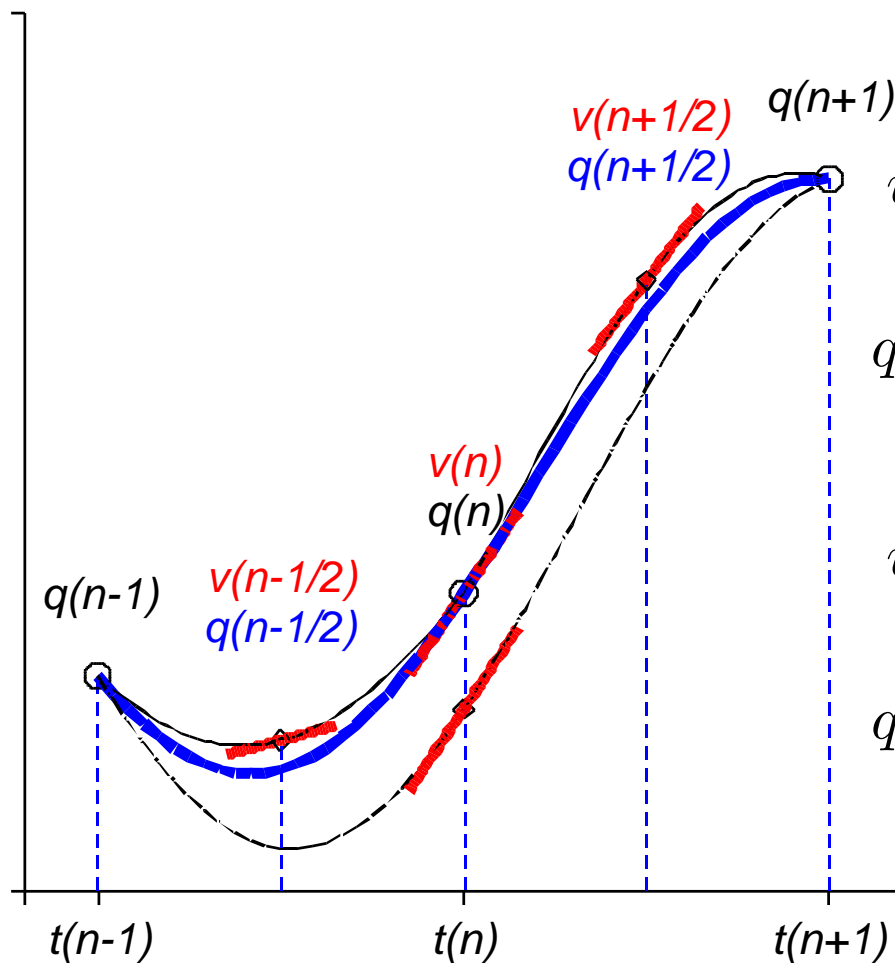$$v(t_n) \approx \dot{p}(t_n) = \frac{1}{\operatorname{sinc} 2\nu} \frac{q_{n+1} - q_{n-1}}{2\,h}$$

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

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

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

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

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

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

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

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

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

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

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

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

S/V$_{\text{EF}}$: one-step formulation

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

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

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

S/V$_{EF}$: one-step formulation

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

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

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

(1) and (2) : $\qquad \dfrac{1}{\operatorname{sinc} \nu} \dfrac{q_{n+1} - q_n}{h} = \cos \nu \, v_n + \dfrac{h}{2} \operatorname{sinc} \nu \; f(q_n)$

S/V$_{EF}$: one-step formulation

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

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

(2) $v_n = \dfrac{1}{\operatorname{sinc} 2\,\nu} \dfrac{q_{n+1} - q_{n-1}}{2\,h}$

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

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

S/V$_{\text{EF}}$: one-step formulation

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

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

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

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

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

S/V$_{\text{EF}}$: one-step formulation

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

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

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

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

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

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

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

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

S/V$_{\text{EF}}$: one-step formulation

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

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

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

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

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

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

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

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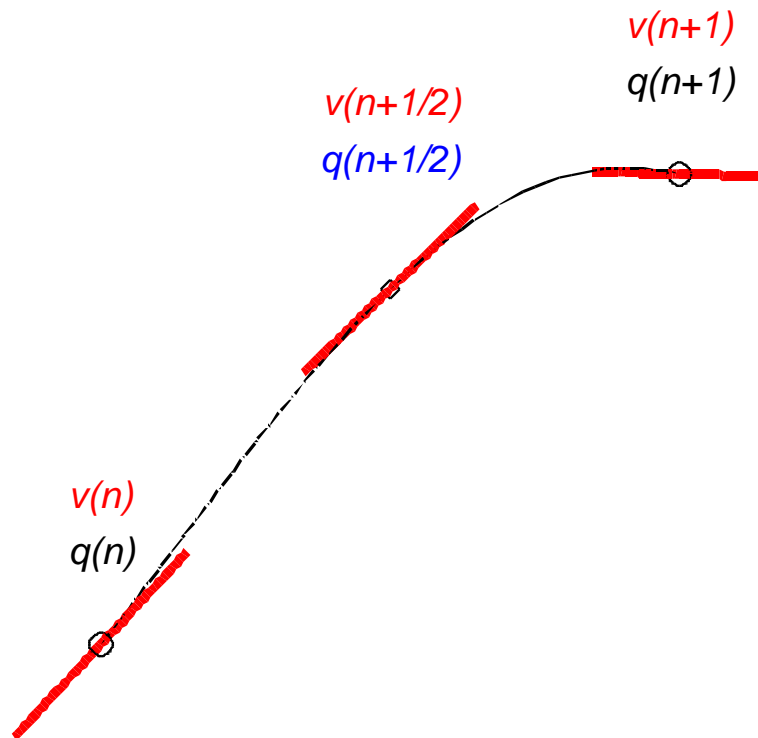
$$\Longleftrightarrow \frac{q_{n+2} - q_n}{2\,h \operatorname{sinc} 2\,\nu} - \frac{q_{n+1} - q_{n-1}}{2\,h \operatorname{sinc} 2\,\nu} = \frac{h}{2} \operatorname{tanc} \nu\, (f(q_n) + f(q_{n+1}))$$

S/V$_{\text{EF}}$: one-step formulation

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

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

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

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

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

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

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

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

$$\Longleftrightarrow \dfrac{q_{n+2} - q_n}{2\,h\operatorname{sinc} 2\,\nu} - \dfrac{q_{n+1} - q_{n-1}}{2\,h\operatorname{sinc} 2\,\nu} = \dfrac{h}{2}\tan\nu\,(f(q_n) + f(q_{n+1}))$$

$$\Longleftrightarrow v_{n+1} - v_n = \dfrac{h}{2}\tan\nu\,(f(q_n) + f(q_{n+1}))$$

S/V$_{EF}$: one-step formulation

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

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

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

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

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

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

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

$$\rule{12cm}{0.4pt}$$

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

$$\Longleftrightarrow \frac{q_{n+2} - q_n}{2\,h \operatorname{sinc} 2\,\nu} - \frac{q_{n+1} - q_{n-1}}{2\,h \operatorname{sinc} 2\,\nu} = \frac{h}{2} \tan c\, \nu\, (f(q_n) + f(q_{n+1}))$$

$$\Longleftrightarrow v_{n+1} - v_n = \frac{h}{2} \tan c\, \nu\, (f(q_n) + f(q_{n+1}))$$

$$v_{n+1} = \frac{1}{\cos \nu} v_{n+\frac{1}{2}} + \frac{h}{2} \tan c\, \nu\, f(q_{n+1})$$

S/V$_{\text{EF}}$: one-step formulation

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

v(n+1)
q(n+1)

v(n+1/2)
q(n+1/2)

v(n)
q(n)

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

EF expl. Euler, $h/2$

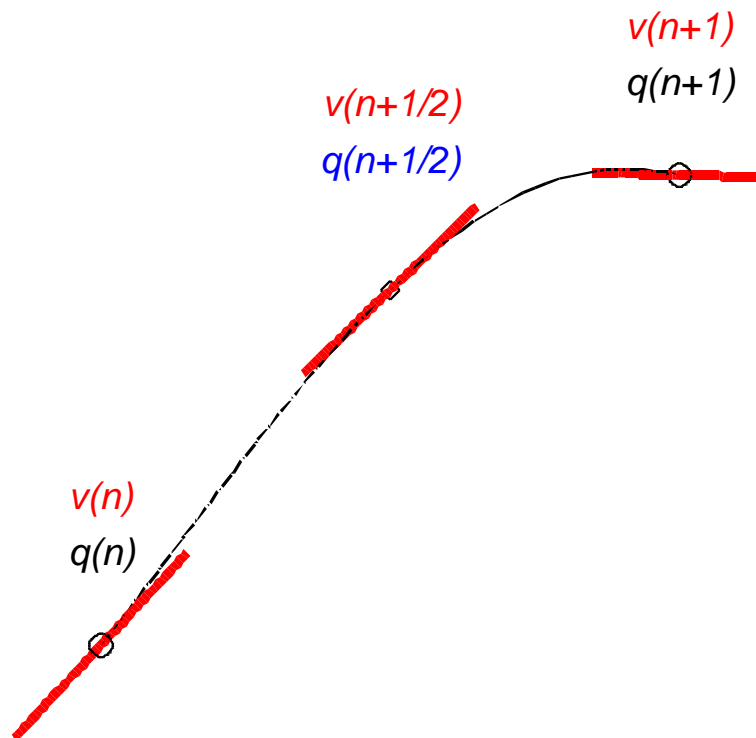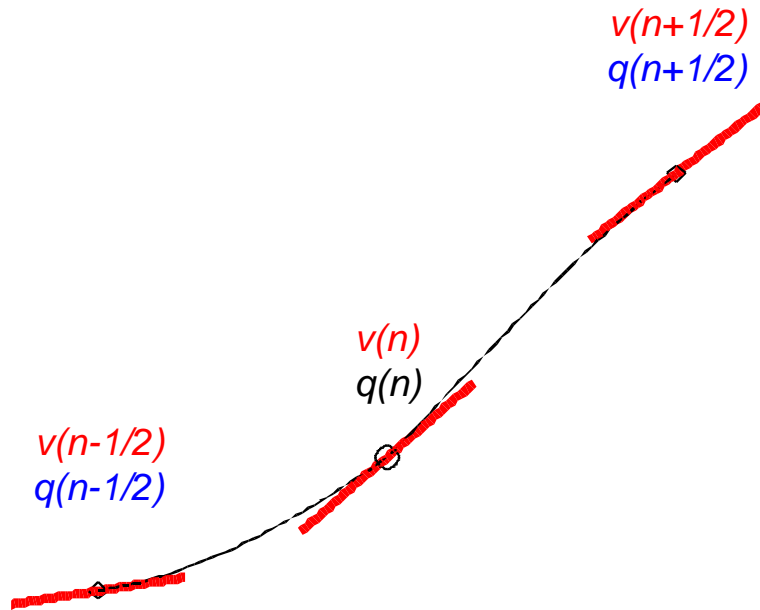$$q_{n+1} = q_n + h\,\mathrm{sinc}\,\nu\, v_{n+\frac{1}{2}}$$

EF expl. midpoint, h

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

EF impl. Euler, $h/2$

S/V$_{\mathbf{EF}}$: one-step formulation

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

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

$v(n+1)$
$q(n+1)$

(A$_{\mathrm{EF}}$)

$v(n+1/2)$
$q(n+1/2)$

$v(n)$
$q(n)$

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

EF expl. Euler, $h/2$

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

EF expl. midpoint, h

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

EF impl. Euler, $h/2$

S/V$_{\text{EF}}$: one-step formulation

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

v(n+1/2)
q(n+1/2)

v(n)
q(n)

v(n-1/2)
q(n-1/2)

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

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$_{\text{EF}}$: one-step formulation

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

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

v(n+1/2)
q(n+1/2)

(B$_{\text{EF}}$)

v(n)
q(n)

v(n-1/2)
q(n-1/2)

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

EF expl. Euler, $h/2$

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

EF expl. midpoint, h

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

EF impl. Euler, $h/2$

S/V$_{\text{EF}}$: one-step formulation

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

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

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

S/V$_{\text{EF}}$: one-step formulation

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

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

$$\begin{cases} q_{n+1} = q_n + h \, \text{sinc} \, \nu \, v_{n+\frac{1}{2}} \\[2mm] v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + h \, \text{sinc} \, \nu \, f(q_n) \end{cases}$$

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

The Störmer-Verlet method

- construction

- one-step formulation

- composition method

S/V$_{\text{EF}}$: composition method

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

$$(\text{A}_{\text{EF}}): \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2em] q_{n+1} = q_n + h\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \\[2em] v_{n+1} = \frac{1}{\cos\nu} v_{n+\frac{1}{2}} + \frac{h}{2}\text{tanc}\nu\, f(q_{n+1}) \end{cases}$$

S/V$_{\text{EF}}$: composition method

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

$$(\text{A}_{\text{EF}}) : \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2mm] q_{n+1} = q_n + h\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \begin{cases} q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\tan\!c\nu\, v_{n+\frac{1}{2}} \\[2mm] q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \end{cases} \\[2mm] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\tan\!c\nu\, f(q_{n+1}) \end{cases}$$

S/V$_{\text{EF}}$: composition method

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

$$(\text{A}_{\text{EF}}) : \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2ex] q_{n+1} = q_n + h\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \quad \begin{cases} q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\tan c\nu\, v_{n+\frac{1}{2}} \\[2ex] q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \end{cases} \\[4ex] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\tan c\nu\, f(q_{n+1}) \end{cases}$$

$$\begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2ex] q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\tan c\nu\, v_{n+\frac{1}{2}} \end{cases}$$

$$\begin{cases} q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \\[2ex] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\tan c\,\nu\, f(q_{n+1}) \end{cases}$$

S/V$_{\text{EF}}$: composition method

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

$$(\text{A}_{\text{EF}}): \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2ex] q_{n+1} = q_n + h\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \begin{cases} q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\,\text{tanc}\nu\, v_{n+\frac{1}{2}} \\[2ex] q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \end{cases} \\[2ex] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\text{tanc}\nu\, f(q_{n+1}) \end{cases}$$

$$(\text{SE1}_{\text{EF}}) \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2ex] q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\,\text{tanc}\nu\, v_{n+\frac{1}{2}} \end{cases}$$

$$(\text{SE2}_{\text{EF}}) \begin{cases} q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \\[2ex] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\text{tanc}\,\nu\, f(q_{n+1}) \end{cases}$$

S/V$_{\text{EF}}$: composition method

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

$$(\text{A}_{\text{EF}}) : \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2mm] q_{n+1} = q_n + h\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \quad \begin{cases} q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\tanc\nu\, v_{n+\frac{1}{2}} \\[2mm] q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \end{cases} \\[2mm] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\tanc\nu\, f(q_{n+1}) \end{cases}$$

$$(\text{SE1}_{\text{EF}}) \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[3mm] q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\tanc\nu\, v_{n+\frac{1}{2}} \end{cases}$$

$$(\text{SE2}_{\text{EF}}) \begin{cases} q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \\[3mm] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\tanc\,\nu\, f(q_{n+1}) \end{cases}$$

$$(\text{A}_{\text{EF}}) = (\text{SE2}_{\text{EF}}) \circ (\text{SE1}_{\text{EF}})$$

S/V$_{EF}$: composition method

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

$$(\text{A}_{EF}): \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[2mm] q_{n+1} = q_n + h\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \quad \begin{cases} q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\,\text{tanc}\nu\, v_{n+\frac{1}{2}} \\[2mm] q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \end{cases} \\[2mm] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\text{tanc}\nu\, f(q_{n+1}) \end{cases}$$

$$(\text{SE1}_{EF}) \begin{cases} v_{n+\frac{1}{2}} = \cos\nu\, v_n + \frac{h}{2}\text{sinc}\,\nu\, f(q_n) \\[3mm] q_{n+\frac{1}{2}} = \frac{1}{\cos\nu}q_n + \frac{h}{2}\,\text{tanc}\nu\, v_{n+\frac{1}{2}} \end{cases}$$

$$(\text{SE2}_{EF}) \begin{cases} q_{n+1} = \cos\nu\, q_{n+\frac{1}{2}} + \frac{h}{2}\,\text{sinc}\,\nu\, v_{n+\frac{1}{2}} \\[3mm] v_{n+1} = \frac{1}{\cos\nu}v_{n+\frac{1}{2}} + \frac{h}{2}\text{tanc}\,\nu\, f(q_{n+1}) \end{cases}$$

$$(\text{A}_{EF}) = (\text{SE2}_{EF})\circ(\text{SE1}_{EF}) \qquad\qquad (\text{B}_{EF}) = (\text{SE1}_{EF})\circ(\text{SE2}_{EF})$$

The Störmer-Verlet method

- construction

- one-step formulation

- composition method

- splitting method

S/V$_{EF}$: splitting method

$$\ddot{q} = f(q)$$

S/V$_{\mathbf{EF}}$: splitting method

$$\ddot{q} = f(q) = g(q) - \omega^2 q \iff \ddot{q} + \omega^2 q = g(q)$$

S/V$_{EF}$: splitting method

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

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

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

S/V$_{EF}$: splitting method

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

Split the vector field

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

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

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

S/V$_{\text{EF}}$: splitting method

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

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

S/V$_{EF}$: splitting method

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

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

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

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

S/V$_{\text{EF}}$: splitting method

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

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

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

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

S/V$_{\text{EF}}$: splitting method

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

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

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

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

$$(\text{SE2}_{\text{EF}}) = \varphi_{\frac{h}{2}\tan\text{c}\,\nu}^{[2]} \circ \varphi_{\frac{h}{2}}^{[1]} \qquad (\text{SE1}_{\text{EF}}) = \varphi_{\frac{h}{2}}^{[1]} \circ \varphi_{\frac{h}{2}\tan\text{c}\,\nu}^{[2]}$$

S/V$_{\text{EF}}$: splitting method

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

$$(\text{A}_{\text{EF}}) = (\text{SE2}_{\text{EF}}) \circ (\text{SE1}_{\text{EF}}) \qquad\qquad (\text{B}_{\text{EF}}) = (\text{SE1}_{\text{EF}}) \circ (\text{SE2}_{\text{EF}})$$
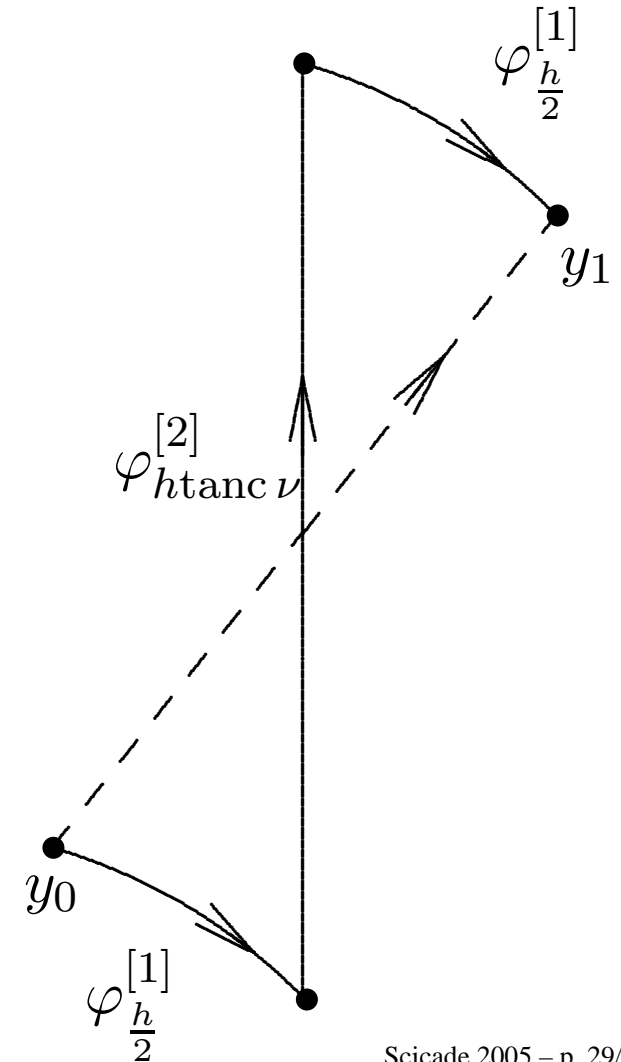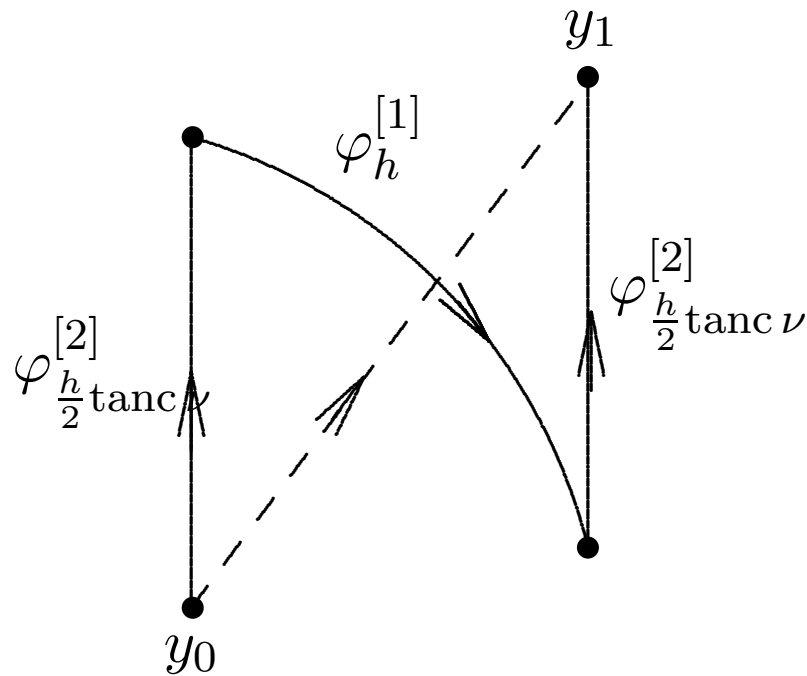
The Störmer-Verlet method

- construction

- one-step formulation

- composition method

- splitting method

- variational integrator

The pendulum

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

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

The pendulum

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

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(A)
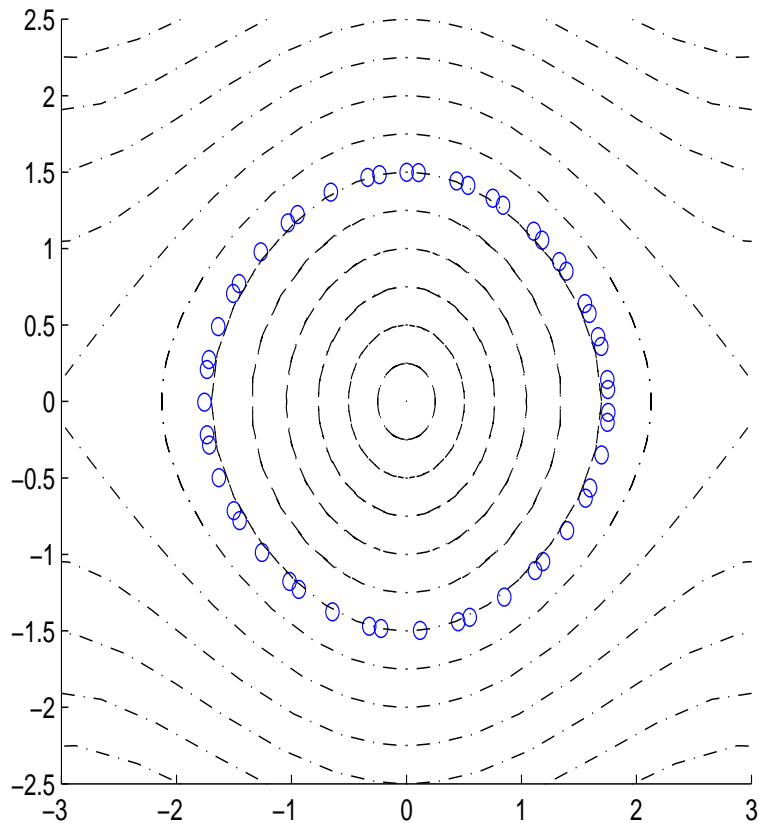
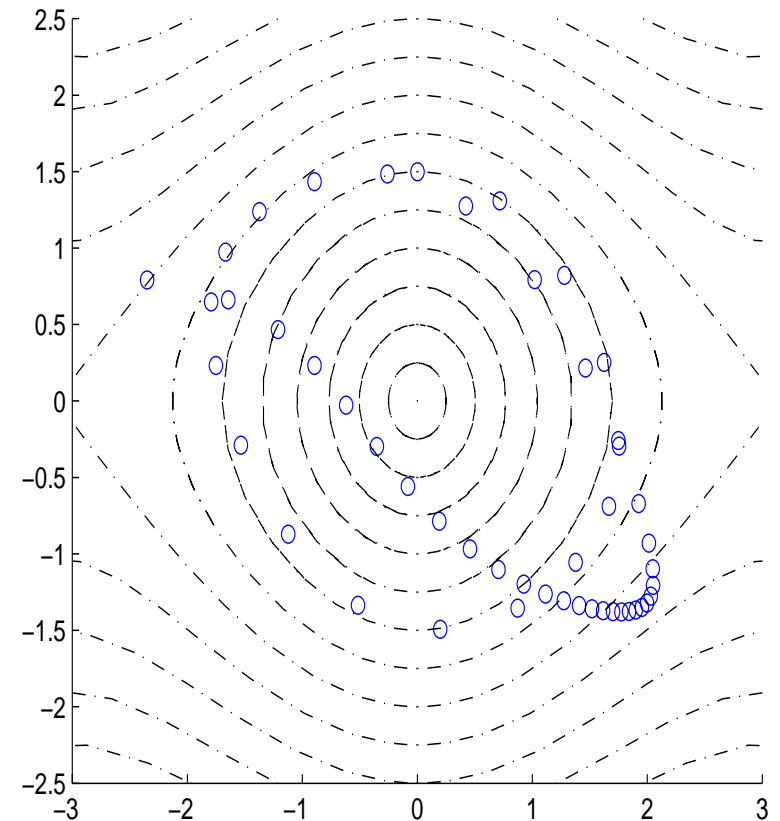# The pendulum

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

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

(A)
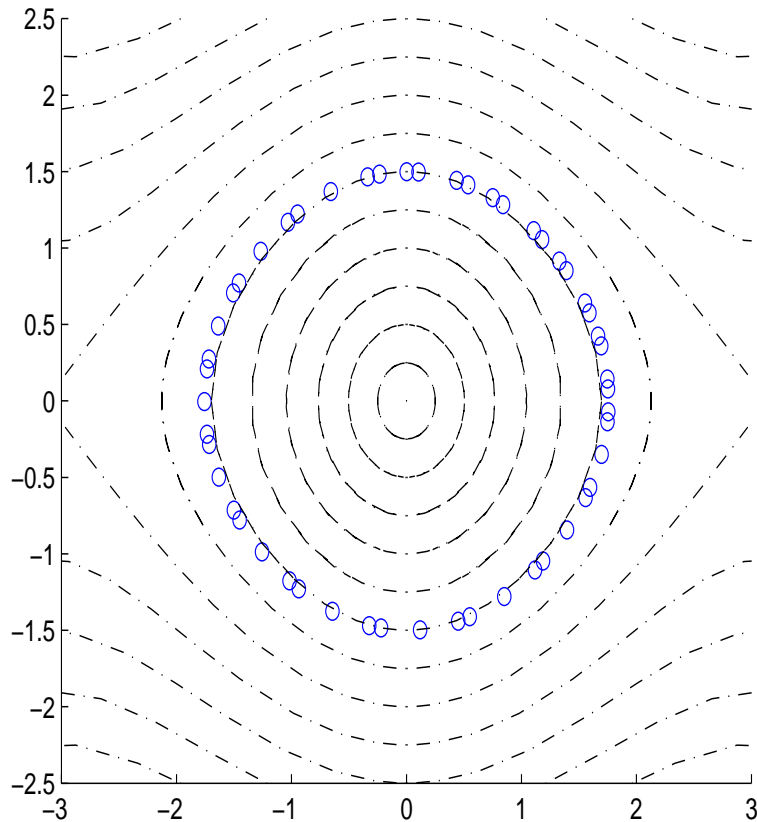
(A_{EF})

$\omega = 1$

The pendulum

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

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

SE1$_{EF}$

SE1

$$\omega = 1$$
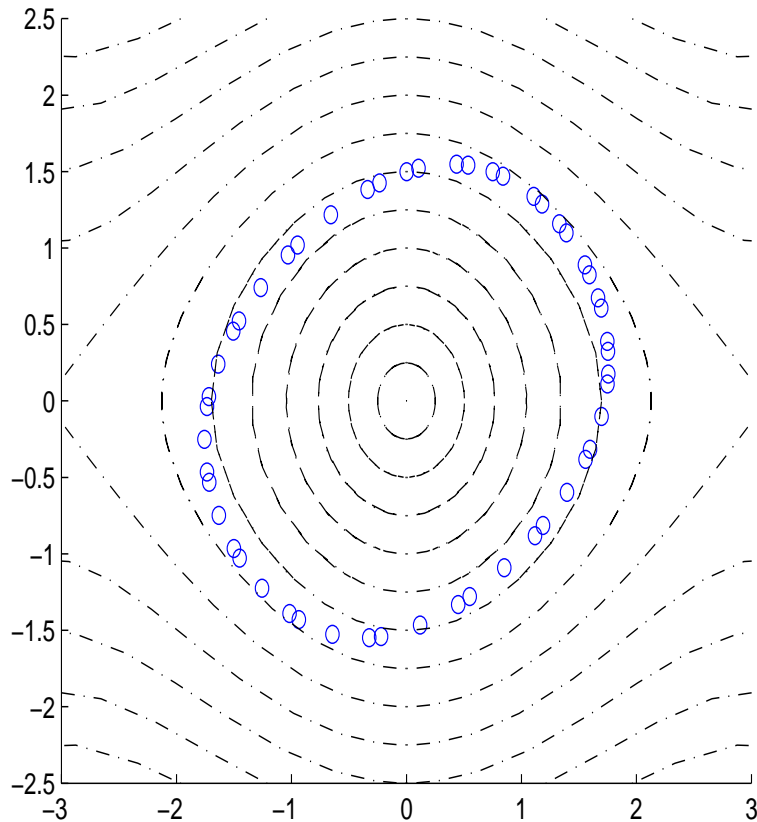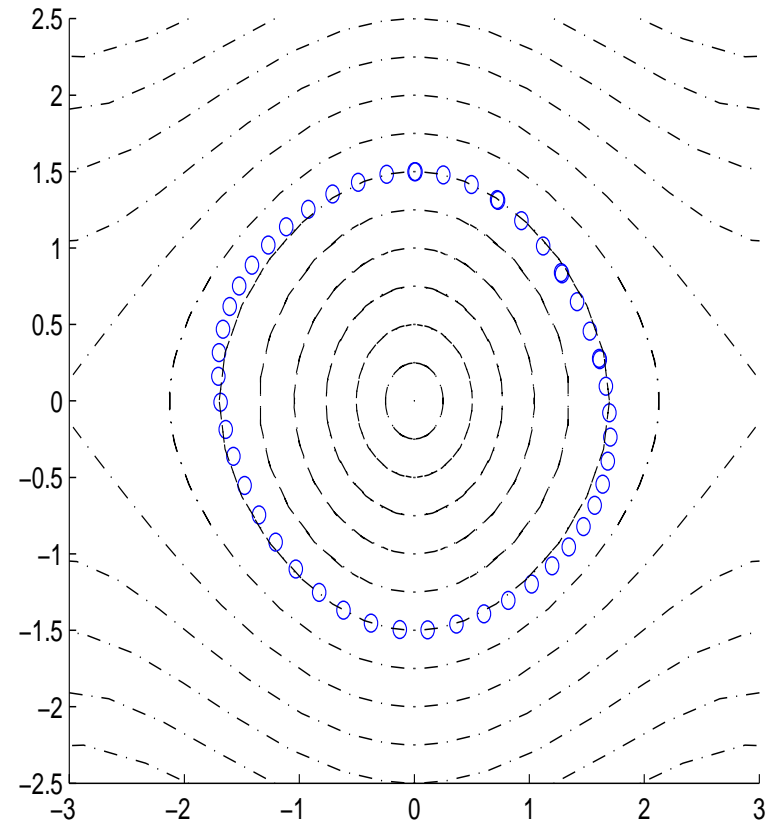
The pendulum

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

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

$$\text{SE1}_{\text{EF}}$$

$$\omega = 1.4$$

The pendulum

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

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

$$\text{SE1}_{\text{EF}} \qquad\qquad\qquad\qquad \text{SE1}_{\text{EF}}$$
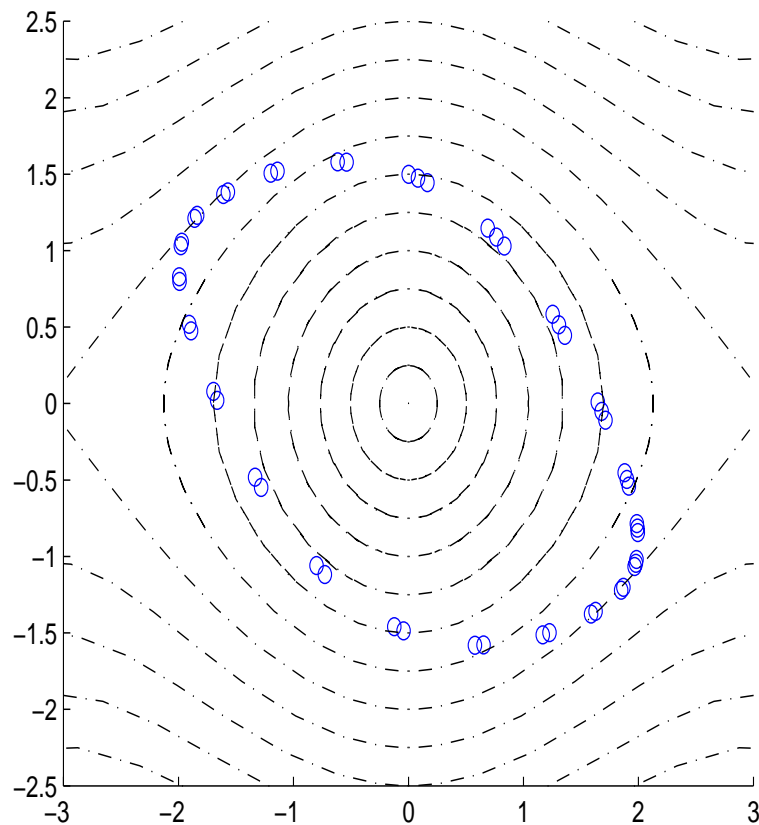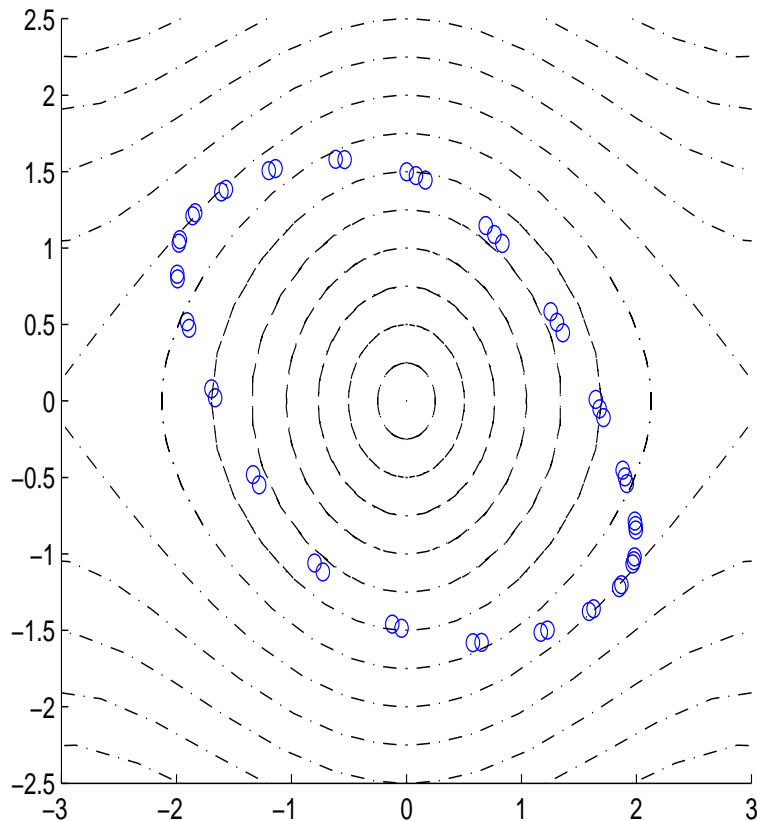
$$\omega = 1.4 \qquad\qquad\qquad\qquad \omega_n = 1 + n/50$$

The Störmer-Verlet method

- construction

- one-step formulation

- composition method

- splitting method

- variational integrator

Example : ω must be held constant

The Störmer-Verlet method

- construction

- one-step formulation

- composition method

- splitting method

- variational integrator

Example : ω must be held constant

- geometric properties

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

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

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

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

The pendulum : symplecticity
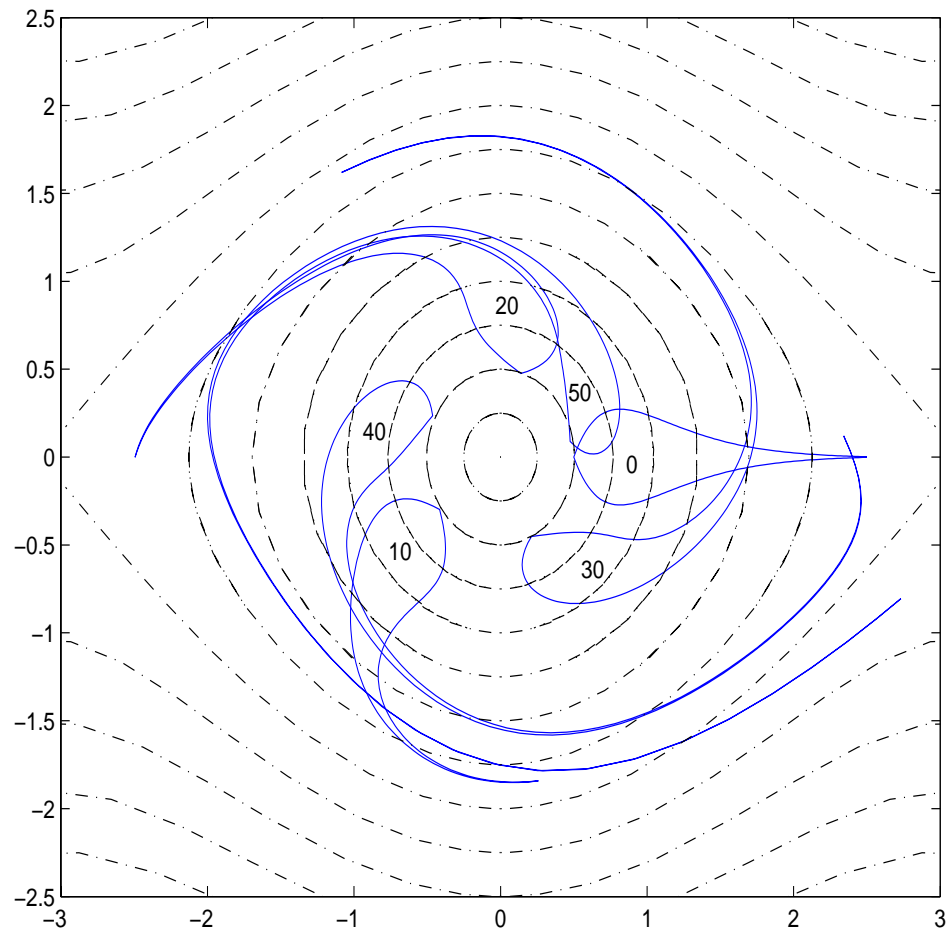
$$\ddot{q} = -\sin q$$

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

SE1
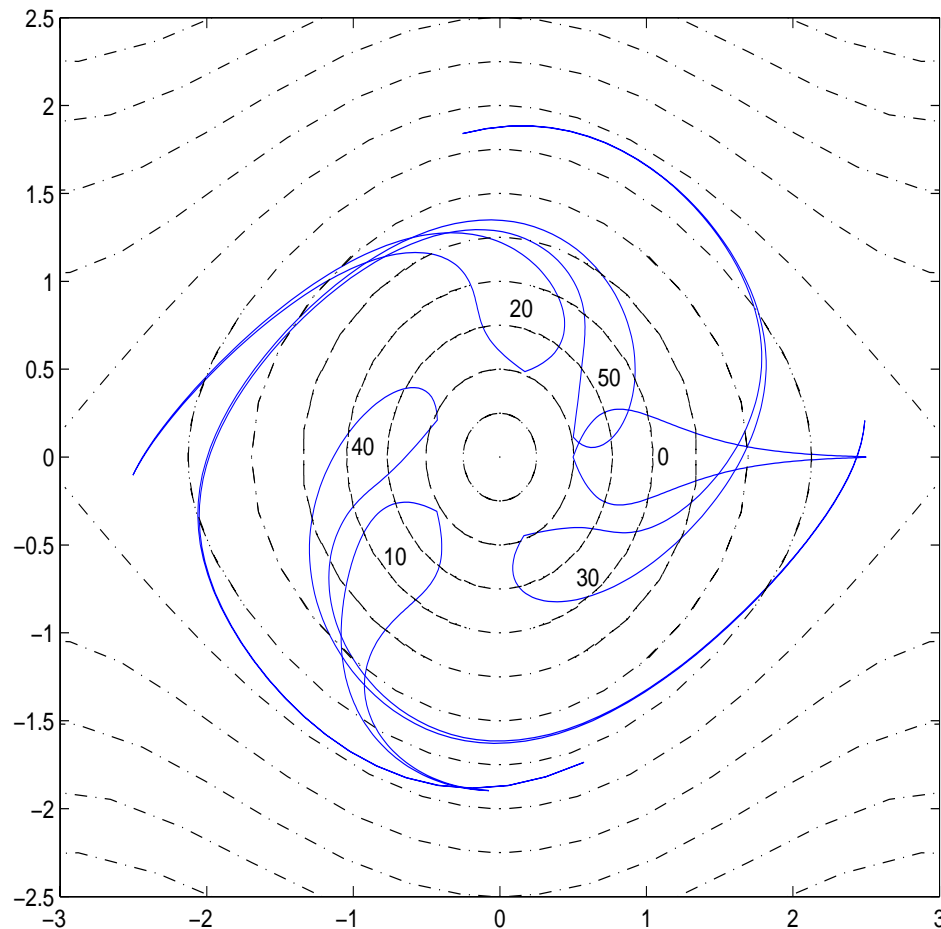
SE1$_{\text{EF}}$
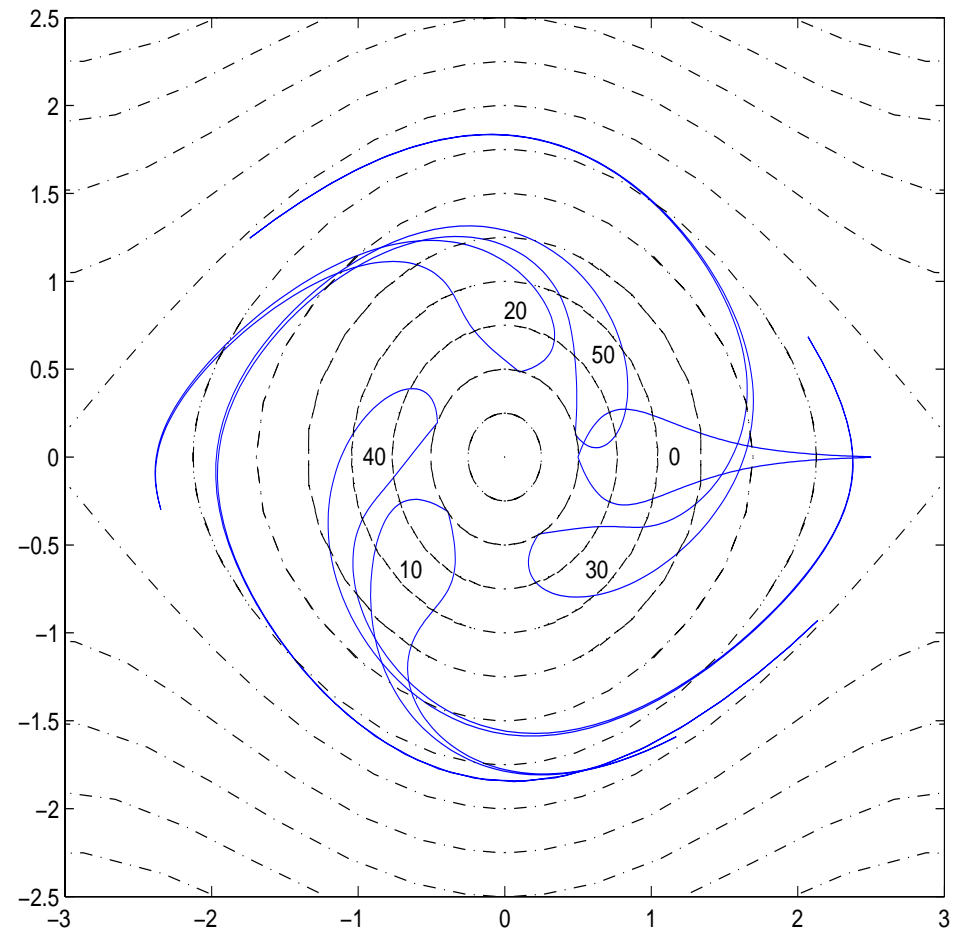
$\omega = 1$

The pendulum : symplecticity

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The pendulum : symplecticity

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

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 ?

Problem

How to obtain a good fixed choice for ω ?

- study of modified equation : backward error analysis

- study of error in H

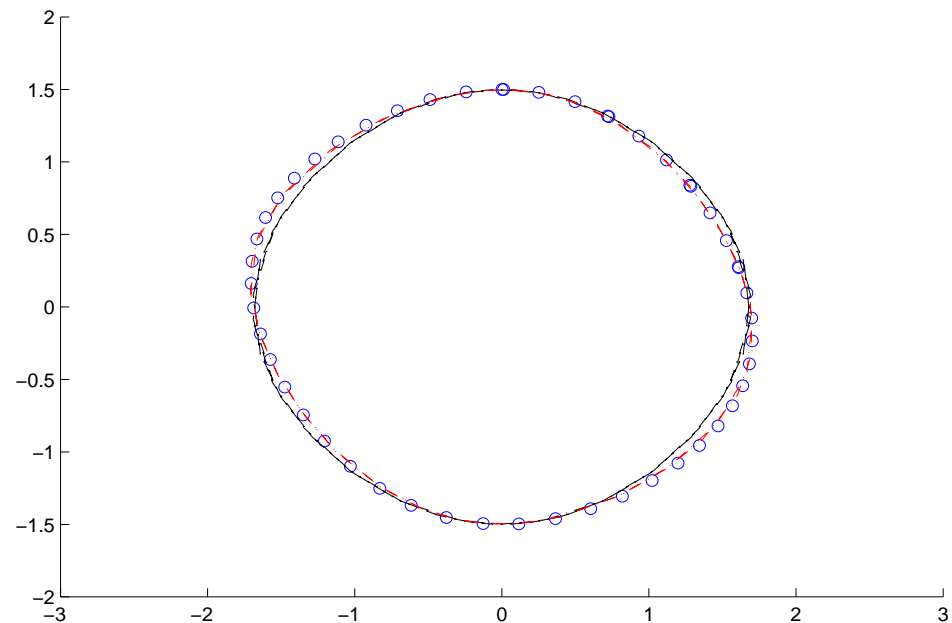# The pendulum : modified eqn.

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

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

SE1
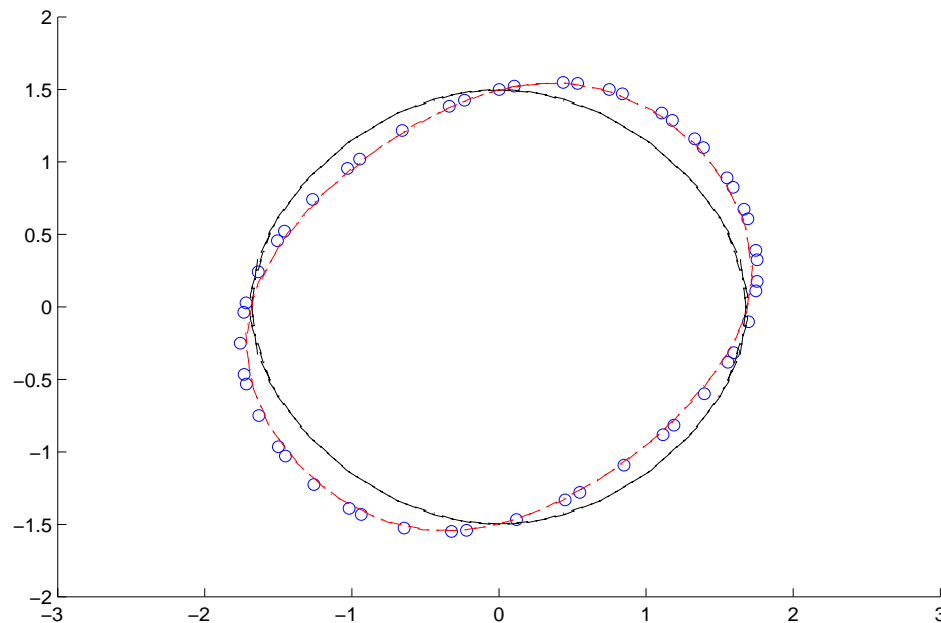
$$\text{SE1}_{\text{EF}}$$

$$\omega = 1$$

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

$$\dot{v} = -\sin q + \frac{h}{2}\left(\cos q - \omega^2\right) + \mathcal{O}(h^2)$$
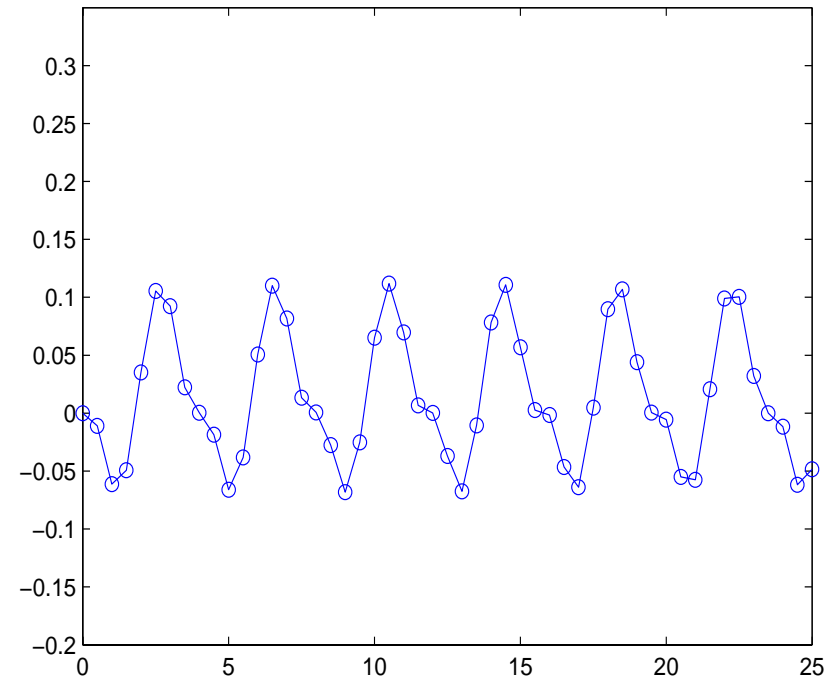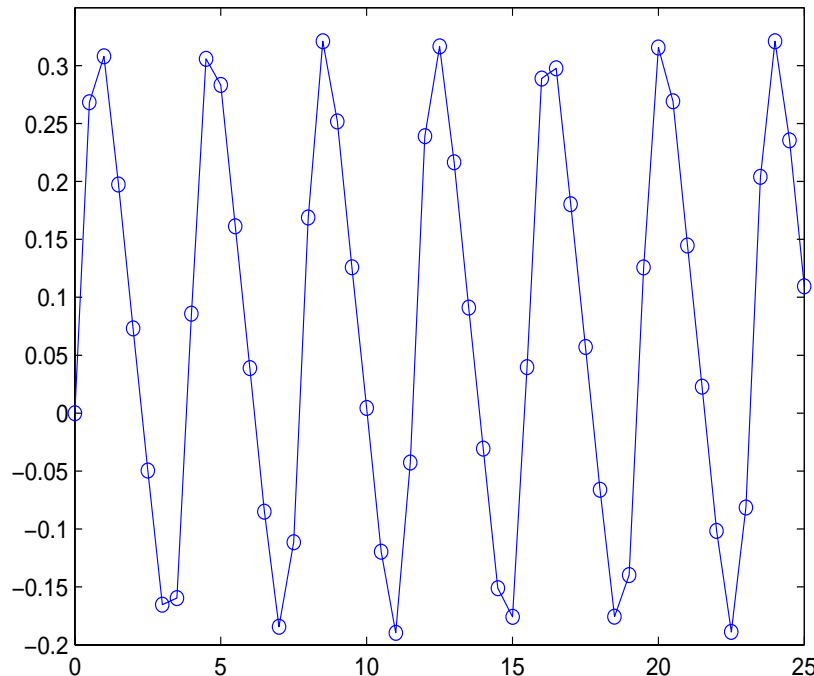
The pendulum : error in H

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

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

SE1

$$\text{SE1}_{\text{EF}}$$

$$\omega = 1$$

$$H_{n+1} = H_n + \left(\frac{1}{2} \sin q_n (\omega^2 q_n - \sin q_n) + \frac{1}{2} p_n^2 (\cos q_n - \omega^2) \right) h^2 + \mathcal{O}(h^3)$$
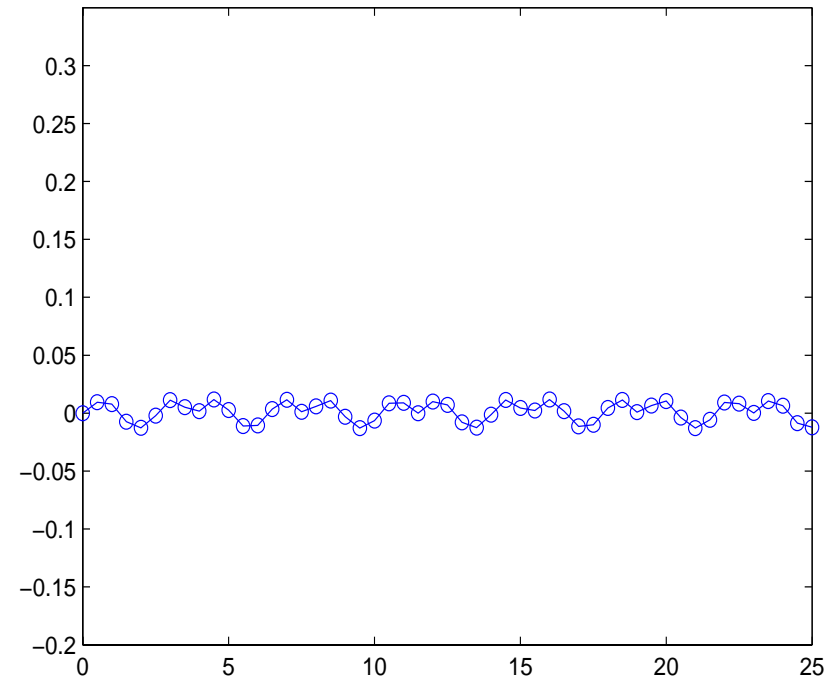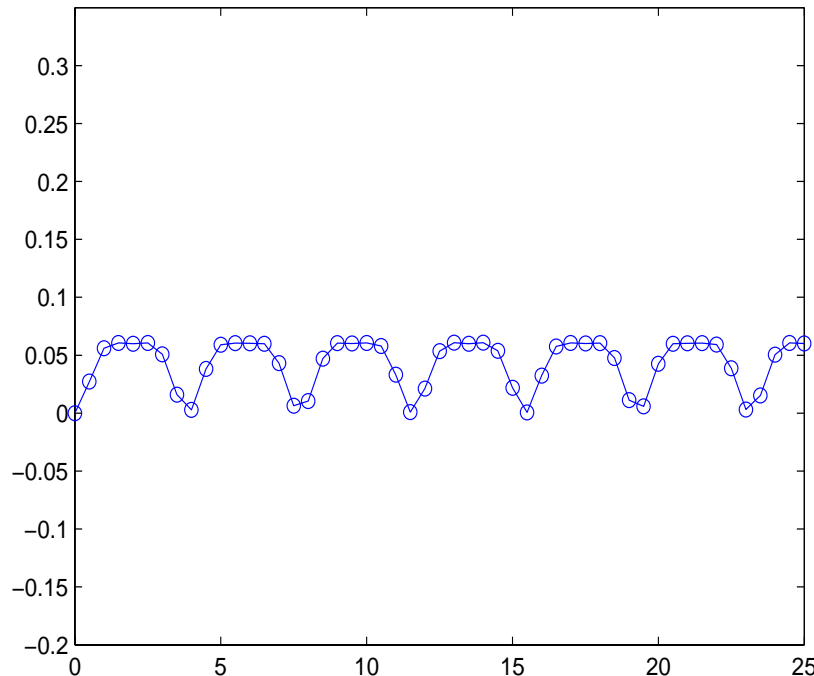
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$$h = 0.5, \, 50 \text{ steps}$$

(A)

(A_{EF})

$\omega = 1$

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

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.