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)

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

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 $t_{n-1},\,t_n,\,t_{n+1}$:

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

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}.

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

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

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

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

Störmer-Verlet method

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

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

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

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

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}.

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

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

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

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

Choice of ω

based on local truncation error

- Störmer-Verlet

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

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

- Numerov

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

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

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

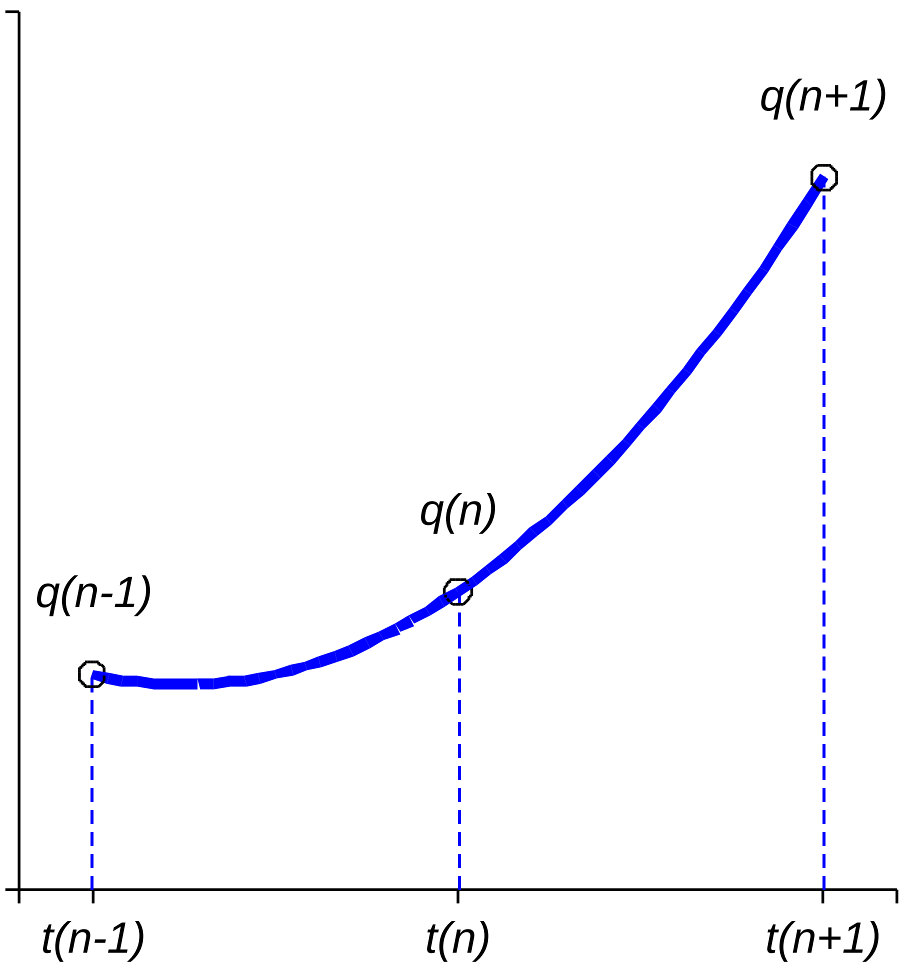
The Störmer-Verlet method

- construction

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

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

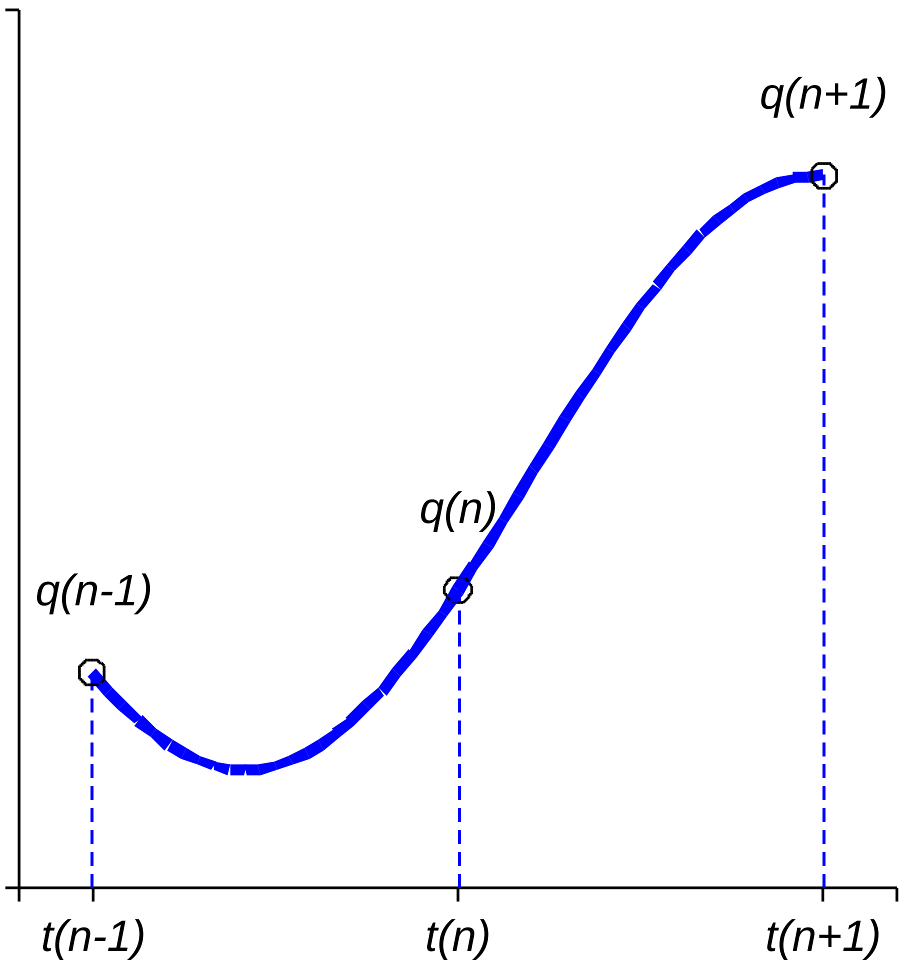
Approximate $\ddot{q}(t_n) = f(q(t_n))$ by $\ddot{p}(t_n) = \dfrac{q_{n+1} - 2\,q_n + q_{n-1}}{h^2}$



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

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



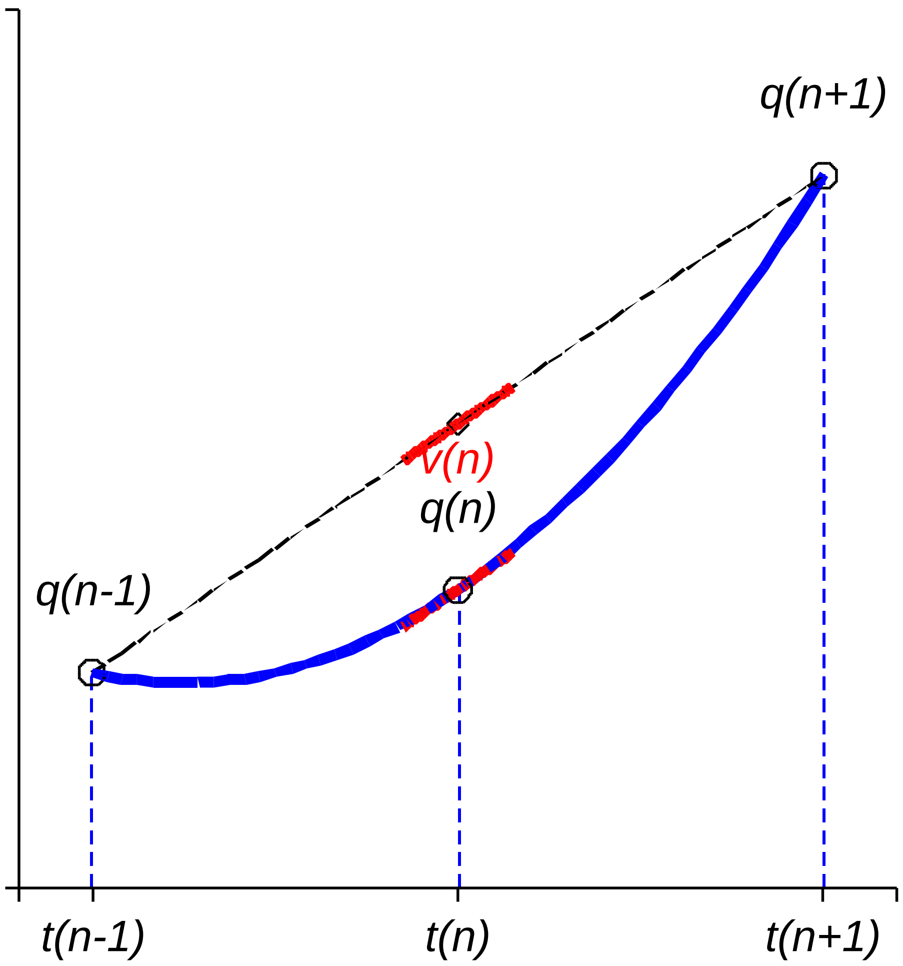
The Störmer-Verlet method

- construction
- one-step formulation

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

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

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



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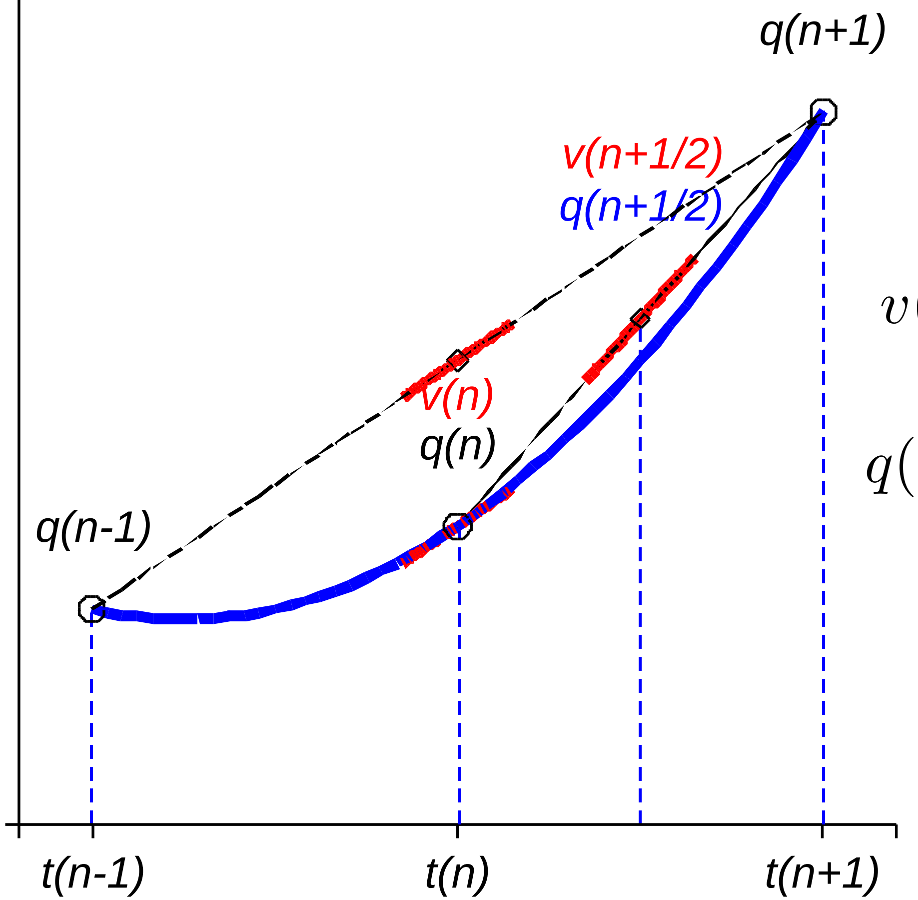

$$v(t_{n+\frac{1}{2}}) \approx \frac{q_{n+1} - q_n}{h}$$

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

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

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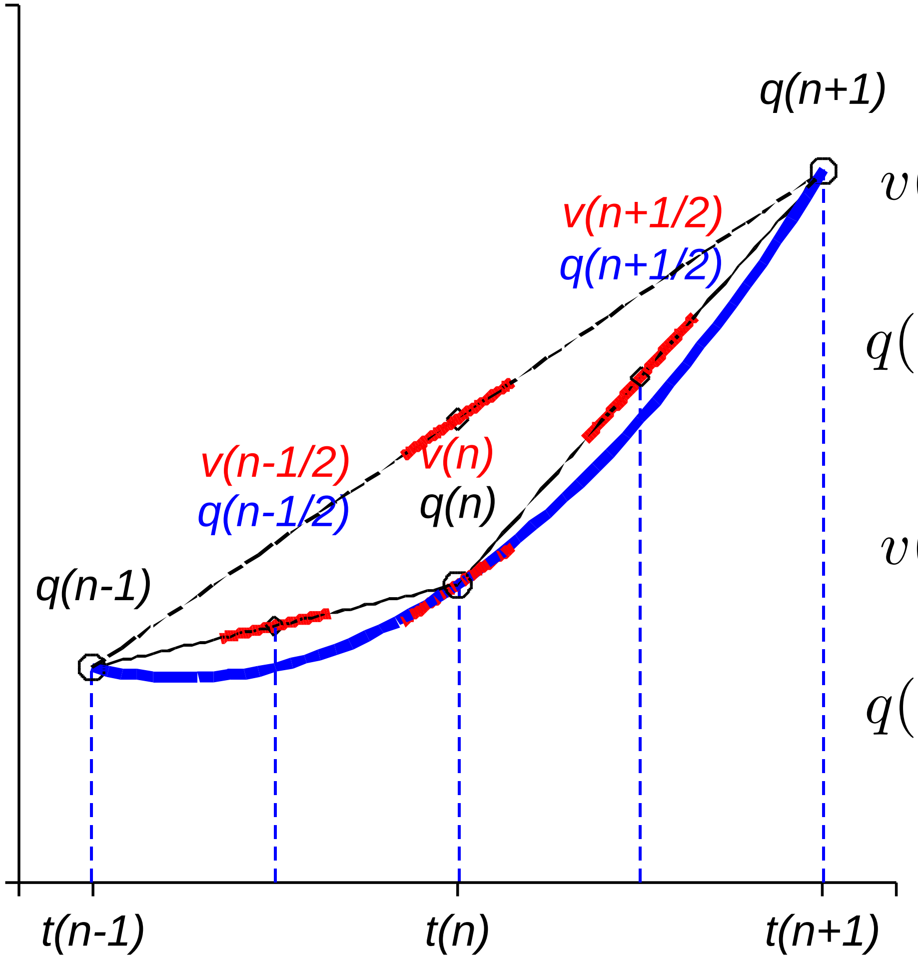


$$v(t_{n+\frac{1}{2}}) \approx \frac{q_{n+1} - q_n}{h}$$

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

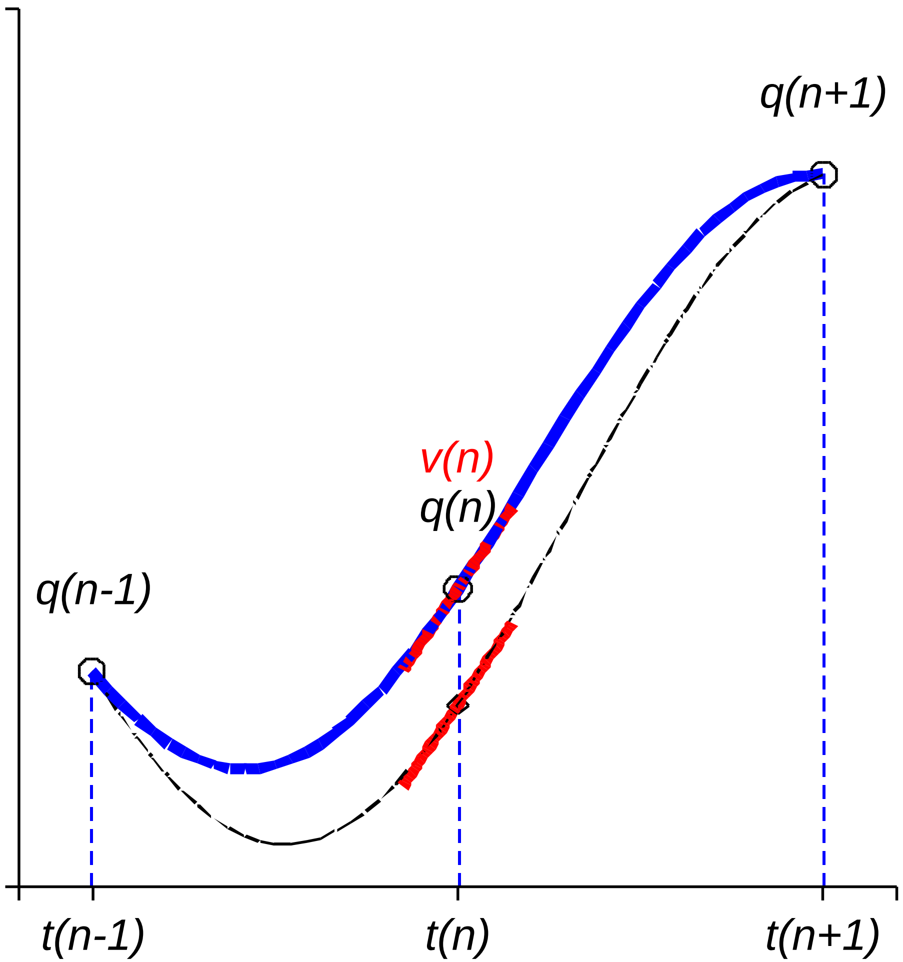
$$v(t_{n-\frac{1}{2}}) \approx \frac{q_n - q_{n-1}}{h}$$

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

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

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

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



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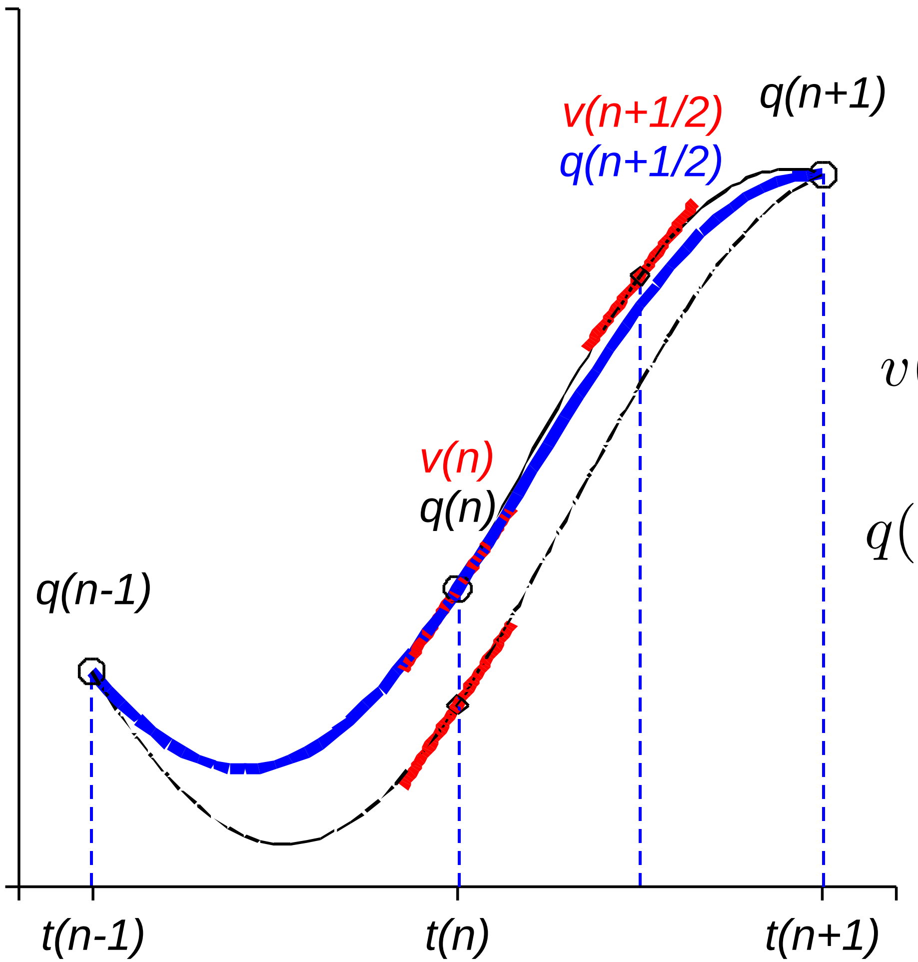


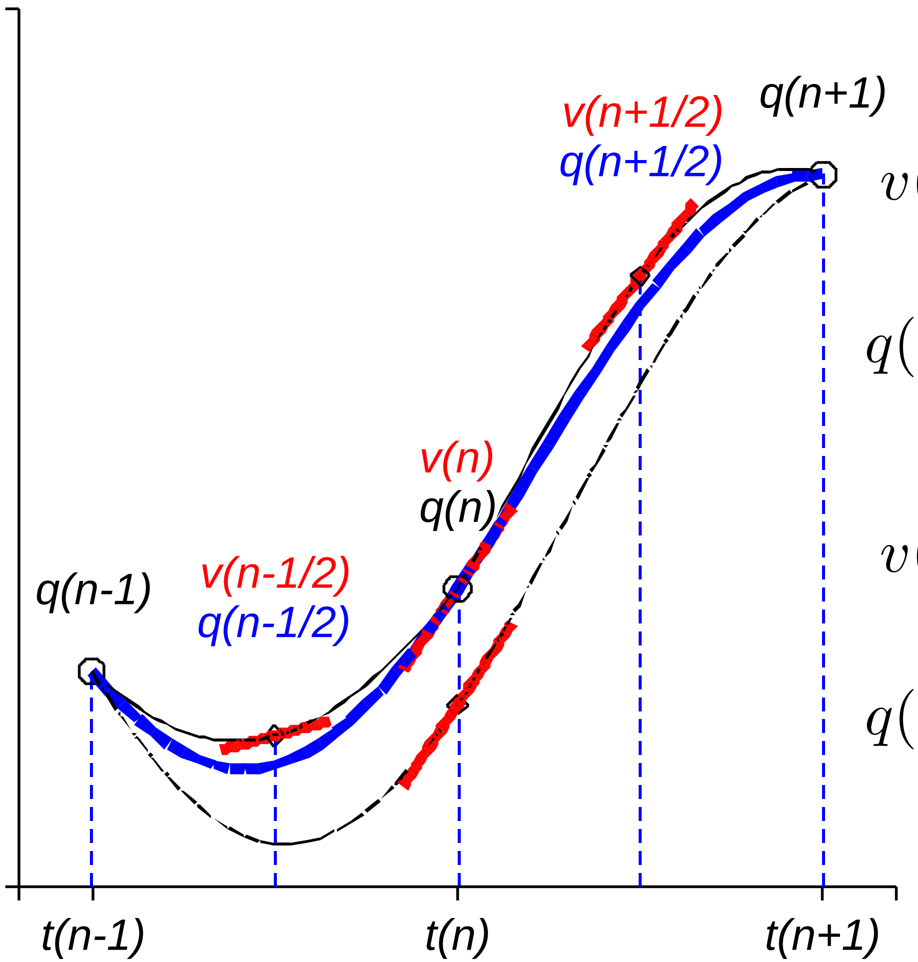
$$v(t_{n+\frac{1}{2}}) \approx \frac{1}{\mathrm{sinc}\,\nu}\,\frac{q_{n+1} - q_n}{h}$$

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

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

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

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



$$v(t_{n+\frac12}) \approx \frac{1}{\mathrm{sinc}\,\nu}\,\frac{q_{n+1} - q_n}{h}$$

$$q(t_{n+\frac12}) \approx \frac{1}{\cos\nu}\,\frac{q_{n+1} + q_n}{2}$$

$$v(t_{n-\frac12}) \approx \frac{1}{\mathrm{sinc}\,\nu}\,\frac{q_n - q_{n-1}}{h}$$

$$q(t_{n-\frac12}) \approx \frac{1}{\cos\nu}\,\frac{q_n + q_{n-1}}{2}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{array}{rl} q_{n+1} - 2\,q_n + q_{n-1} & = h^2\,\mathrm{sinc}^2\nu\, f(q_n) \\ +\quad q_{n+2} - 2\,q_{n+1} + \quad q_n & = h^2\,\mathrm{sinc}^2\nu\, f(q_{n+1}) \\ \hline q_{n+2} - \quad q_{n+1} - \quad q_n + q_{n-1} & = h^2\,\mathrm{sinc}^2\nu\,(f(q_n) + f(q_{n+1})) \end{array}$$

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

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

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

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

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

$$\begin{array}{rcl} q_{n+1} - 2\,q_n + q_{n-1} & = & h^2\,\mathrm{sinc}^2\nu\, f(q_n) \\ + \quad q_{n+2} - 2\,q_{n+1} + \quad q_n & = & h^2\,\mathrm{sinc}^2\nu\, f(q_{n+1}) \\ \hline q_{n+2} - \quad q_{n+1} - \quad q_n + q_{n-1} & = & h^2\,\mathrm{sinc}^2\nu\,(f(q_n) + f(q_{n+1})) \end{array}$$

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

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

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

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

(2) $v_n = \dfrac{1}{\mathrm{sinc}\,2\,\nu}\dfrac{q_{n+1}-q_{n-1}}{2\,h}$ (3) $v_{n+\frac12} = \dfrac{1}{\mathrm{sinc}\,\nu}\dfrac{q_{n+1}-q_n}{h}$

(1) and (2) : $v_{n+\frac12} = \dfrac{1}{\mathrm{sinc}\ \nu}\dfrac{q_{n+1}-q_n}{h} = \cos\nu\, v_n + \dfrac{h}{2}\,\mathrm{sinc}\,\nu\, f(q_n)$

$$v_{n+\frac12} = \cos\nu\, v_n + \frac{h}{2}\,\mathrm{sinc}\ \nu\, f(q_n) \qquad q_{n+1} = q_n + h\ \mathrm{sinc}\,\nu\, v_{n+\frac12}$$

$$\begin{array}{rcl}
q_{n+1} - 2\,q_n + q_{n-1} & = & h^2\,\mathrm{sinc}^2\nu\, f(q_n) \\
+ \quad q_{n+2} - 2\,q_{n+1} + \quad q_n & = & h^2\,\mathrm{sinc}^2\nu\, f(q_{n+1}) \\
\hline
q_{n+2} - \quad q_{n+1} - \quad q_n + q_{n-1} & = & h^2\,\mathrm{sinc}^2\nu\,(f(q_n) + f(q_{n+1}))
\end{array}$$

$$\begin{array}{rcl}
\Longleftrightarrow \dfrac{q_{n+2}-q_n}{2\,h\,\mathrm{sinc}\,2\,\nu} - \dfrac{q_{n+1}-q_{n-1}}{2\,h\,\mathrm{sinc}\,2\,\nu} & = & \dfrac{h}{2}\,\mathrm{tanc}\,\nu\,(f(q_n)+f(q_{n+1})) \\
\Longleftrightarrow v_{n+1} - v_n & = & \dfrac{h}{2}\,\mathrm{tanc}\,\nu\,(f(q_n)+f(q_{n+1}))
\end{array}$$

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

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

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

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

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

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

$$\begin{array}{rcl} q_{n+1} - 2\,q_n + q_{n-1} & = & h^2\,\mathrm{sinc}^2\nu\, f(q_n) \\ +\quad q_{n+2} - 2\,q_{n+1} + \quad q_n & = & h^2\,\mathrm{sinc}^2\nu\, f(q_{n+1}) \\ \hline q_{n+2} - \quad q_{n+1} - \quad q_n + q_{n-1} & = & h^2\,\mathrm{sinc}^2\nu\,(f(q_n) + f(q_{n+1})) \end{array}$$

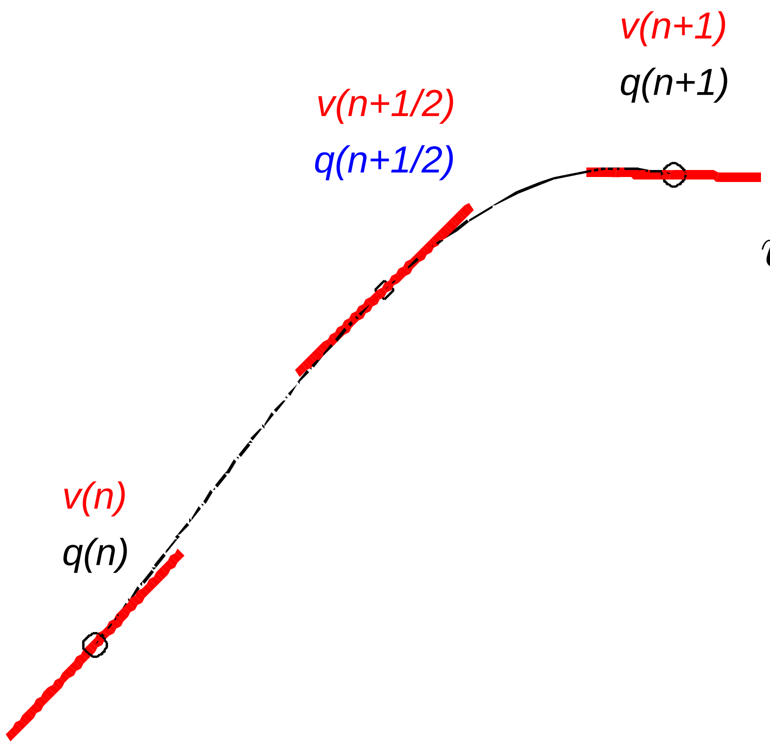
$$\iff \frac{q_{n+2}-q_n}{2\,h\,\mathrm{sinc}\,2\,\nu} - \frac{q_{n+1}-q_{n-1}}{2\,h\,\mathrm{sinc}\,2\,\nu} = \frac{h}{2}\,\mathrm{tanc}\,\nu\,(f(q_n)+f(q_{n+1}))$$

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

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

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

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



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

EF expl. Euler, $h/2$

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

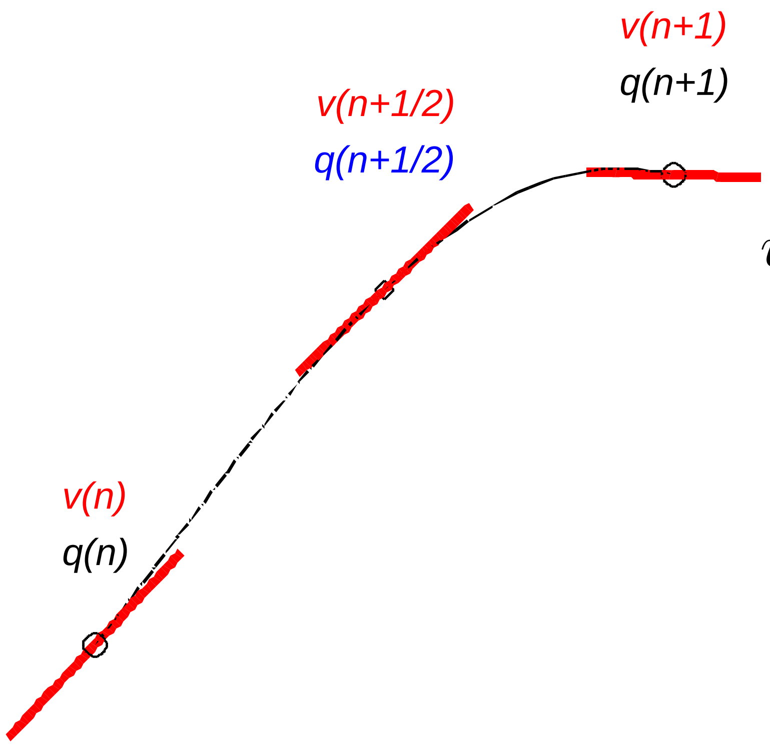
EF expl. midpoint, h

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

EF impl. Euler, $h/2$

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

$$\dot{q} = v \qquad \dot{v} = f(q)$$
$$\Phi_h^A : (q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$$



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

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

EF expl. Euler, $h/2$

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

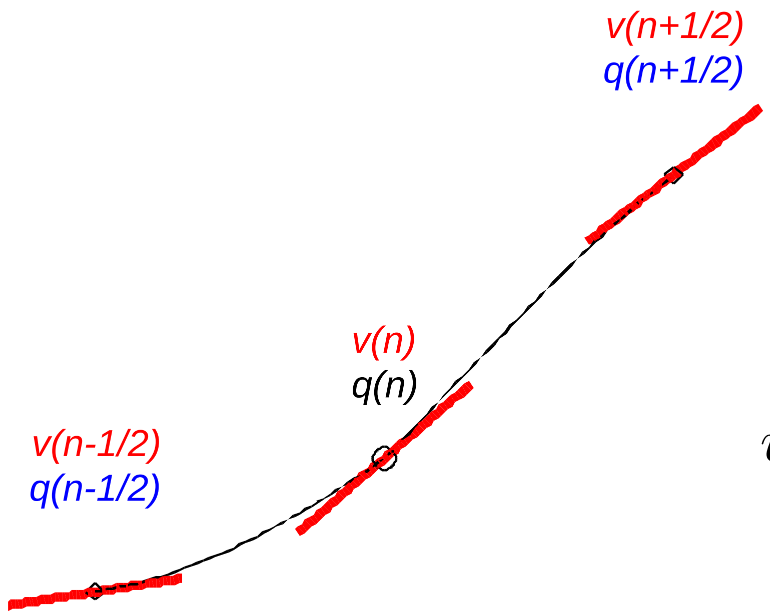
EF expl. midpoint, h

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

EF impl. Euler, $h/2$

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

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



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

EF expl. Euler, $h/2$

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

EF expl. midpoint, h

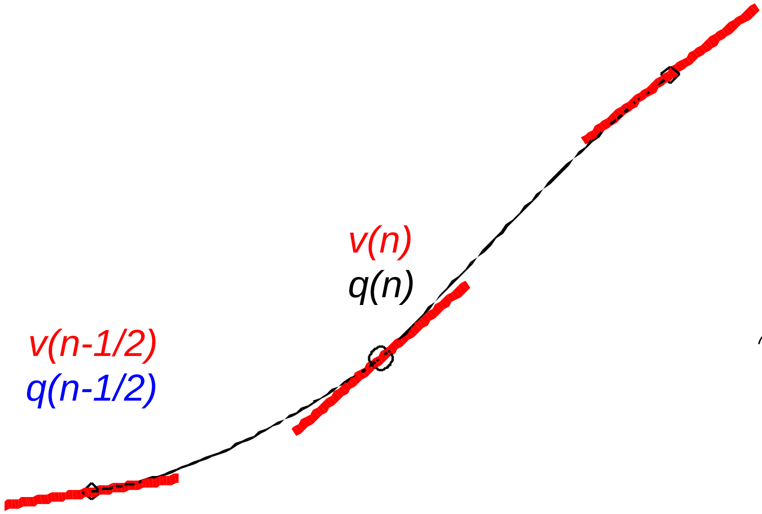
$$q_{n+\frac{1}{2}} = \frac{1}{\cos\nu} q_n + \frac{h}{2}\mathrm{tanc}\nu\, v_{n+\frac{1}{2}}$$

EF impl. Euler, $h/2$

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

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

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



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

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

EF expl. Euler, $h/2$

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

EF expl. midpoint, h

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

EF impl. Euler, $h/2$

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

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

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

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

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

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

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

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

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

The Störmer-Verlet method

- construction
- one-step formulation
- composition method

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

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

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

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

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

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

$\mathbf{S/V_{EF}}$: composition method

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The Störmer-Verlet method

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

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

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

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

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

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

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

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

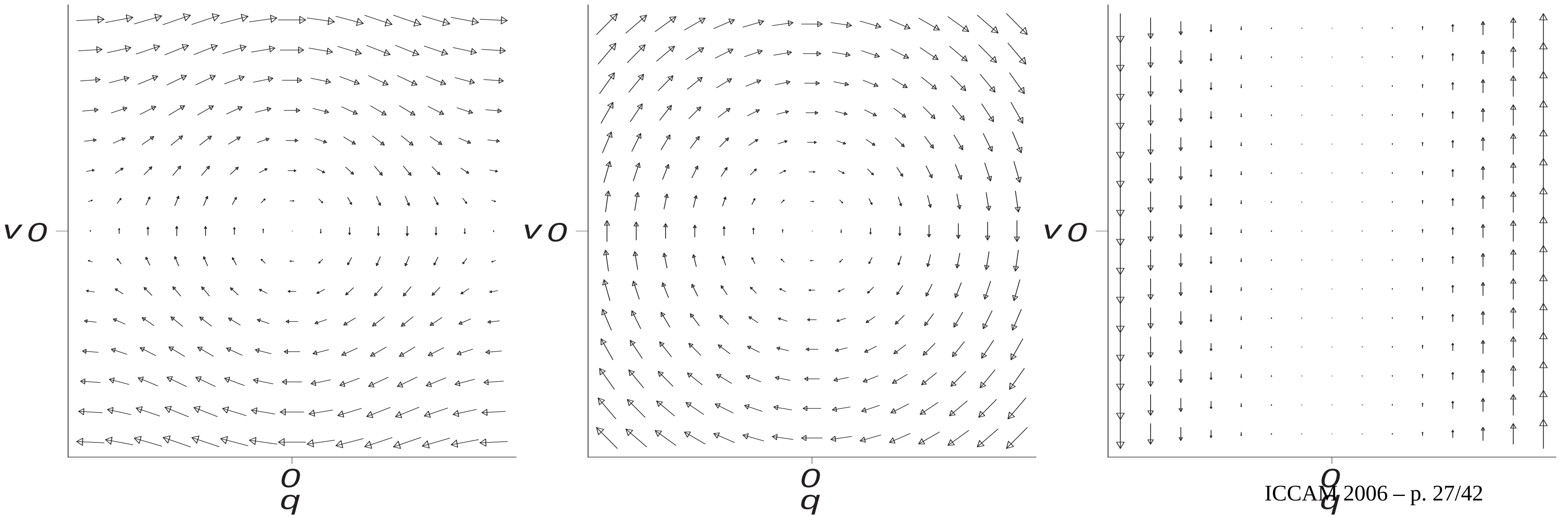
$$\ddot{q} = f(q) = g(q) - \omega^2 q \Longleftrightarrow \ddot{q} + \omega^2 q = g(q) \Longleftrightarrow \begin{cases} \dot{q} = v \\ \dot{v} = g(q) - \omega^2 q \end{cases}$$

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$_{\mathbf{EF}}$: 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$_{\mathbf{EF}}$: 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

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

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

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

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

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$$(\mathrm{SE2_{EF}}) = \varphi^{[2]}_{\frac{h}{2}\mathrm{tanc}\,\nu} \circ \varphi^{[1]}_{\frac{h}{2}} \qquad (\mathrm{SE1_{EF}}) = \varphi^{[1]}_{\frac{h}{2}} \circ \varphi^{[2]}_{\frac{h}{2}\mathrm{tanc}\,\nu}$$

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

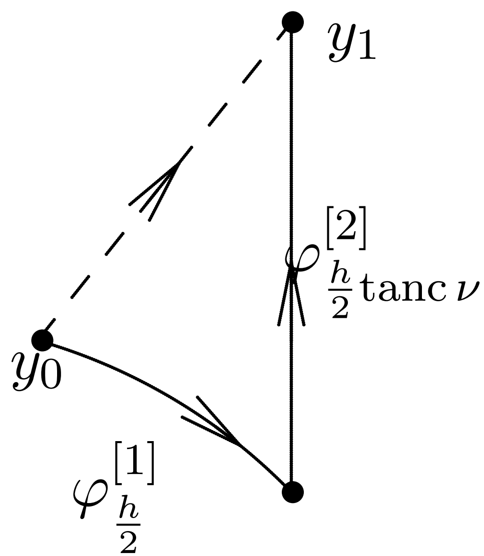
$$\dot{q} = v \qquad \dot{v} = g(q) - \omega^2 q = f(q)$$

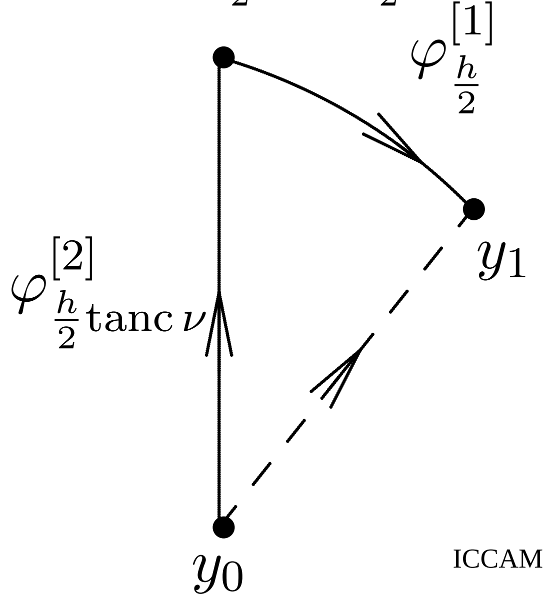
$$(v, g(q) - \omega^2 q) \quad = \quad (v, -\omega^2 q) \quad + \quad (0, g(q))$$

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

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

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

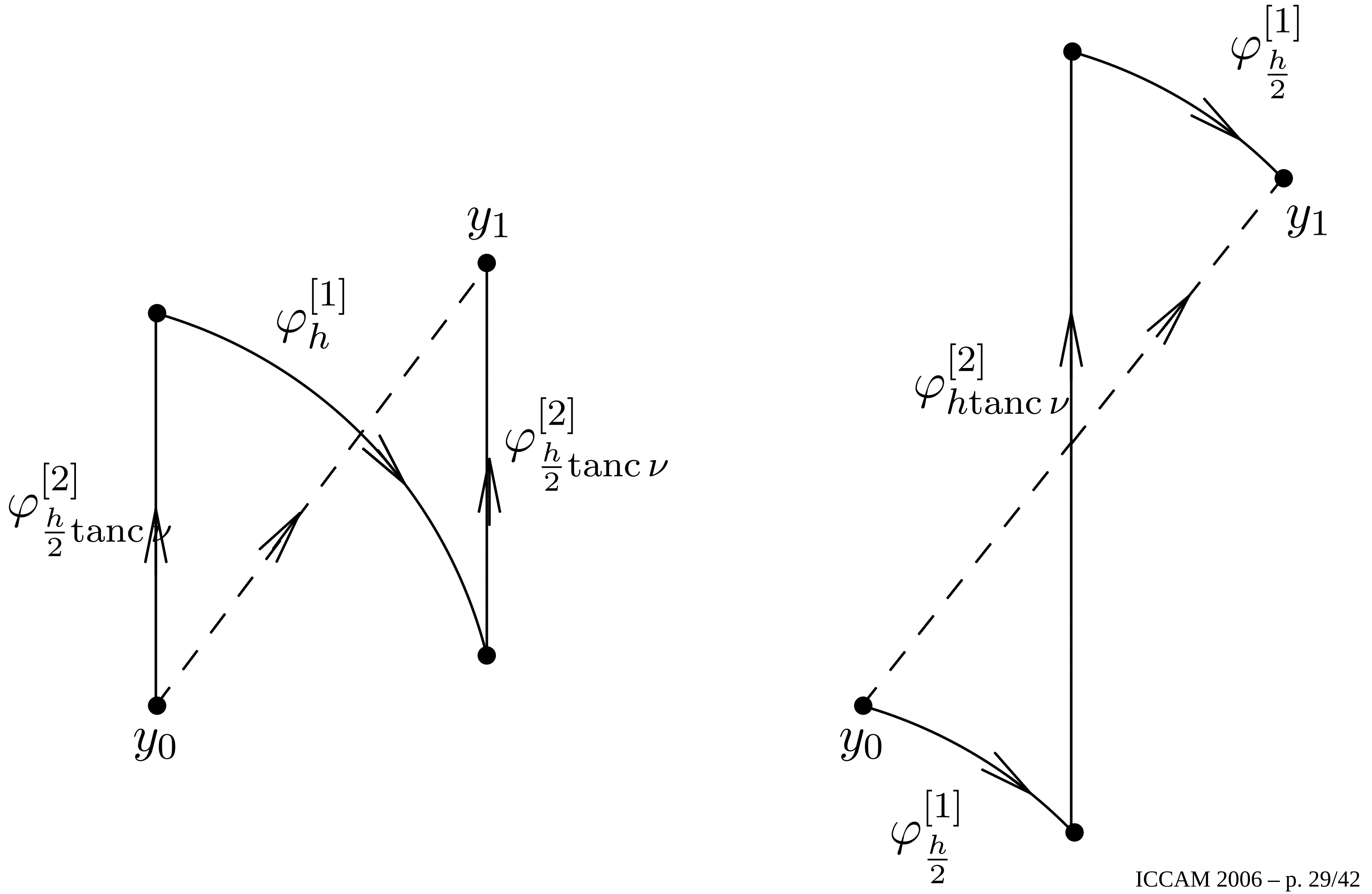




S/V$_{\mathbf{EF}}$: splitting method

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

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



The Störmer-Verlet method

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

The pendulum

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

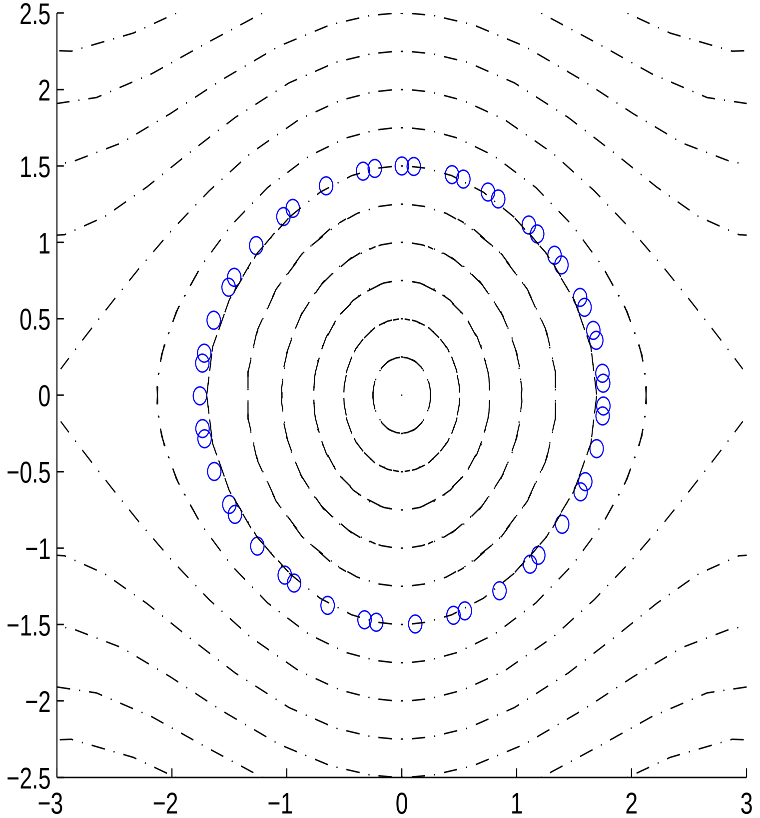
$h = 0.5$, 50 steps

The pendulum

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

$h = 0.5$, 50 steps

(A)

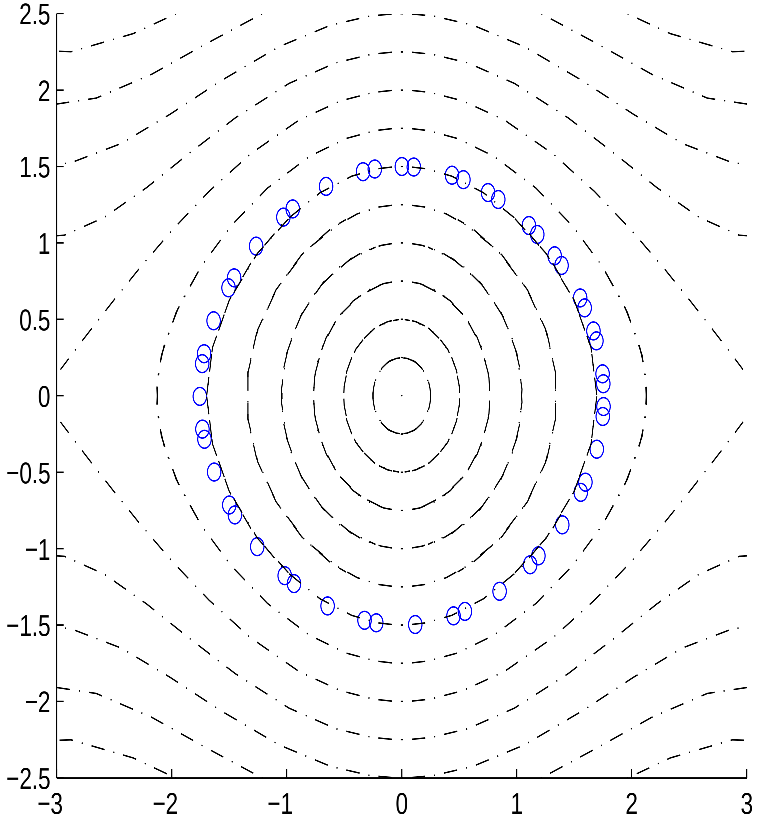


The pendulum

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

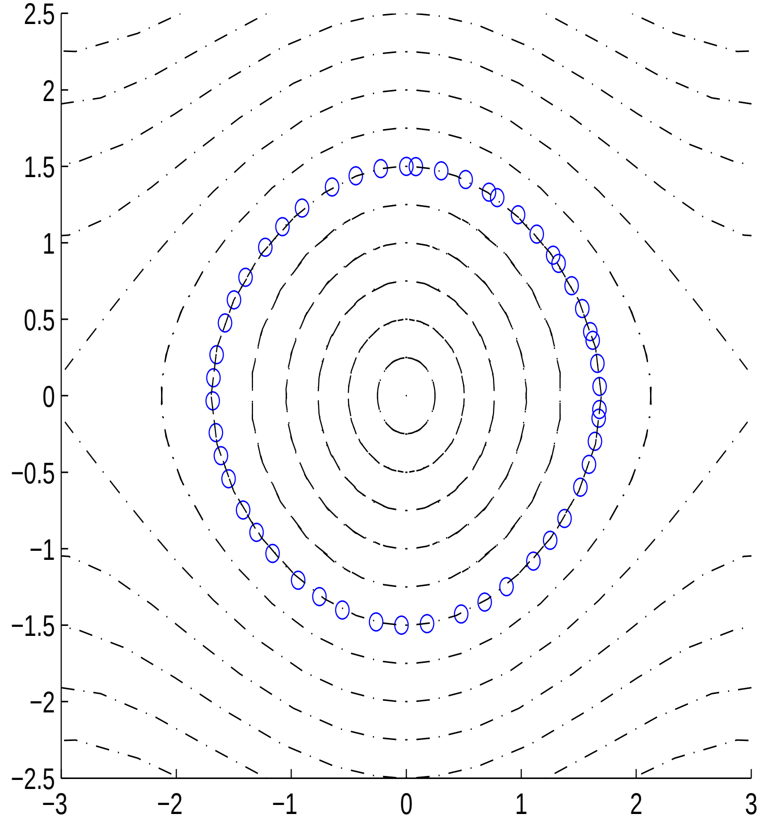
$h = 0.5$, 50 steps

(A)



(A_{EF})

$\omega = 1$

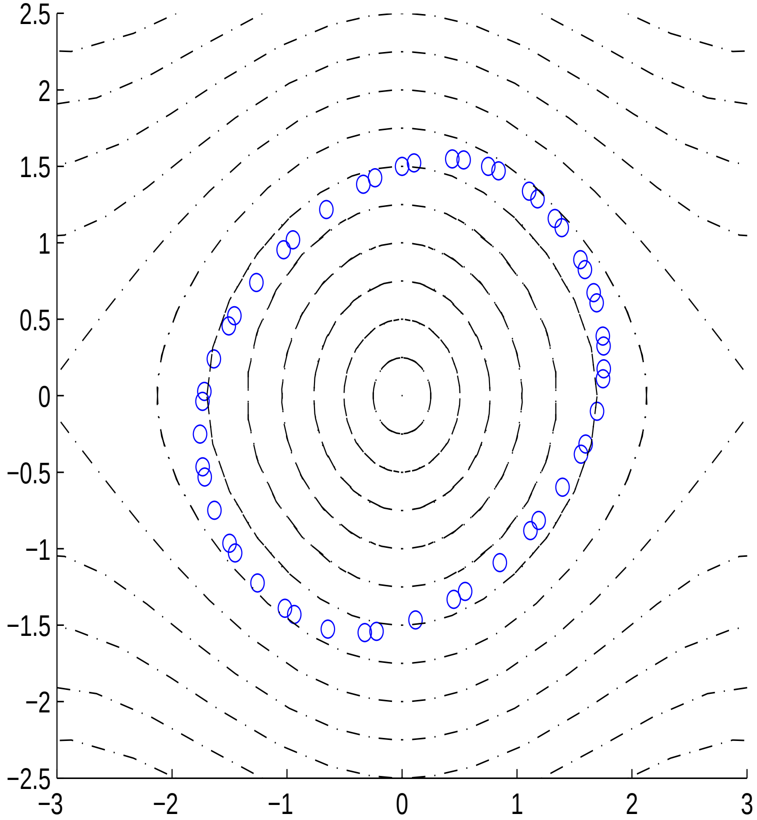


The pendulum

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

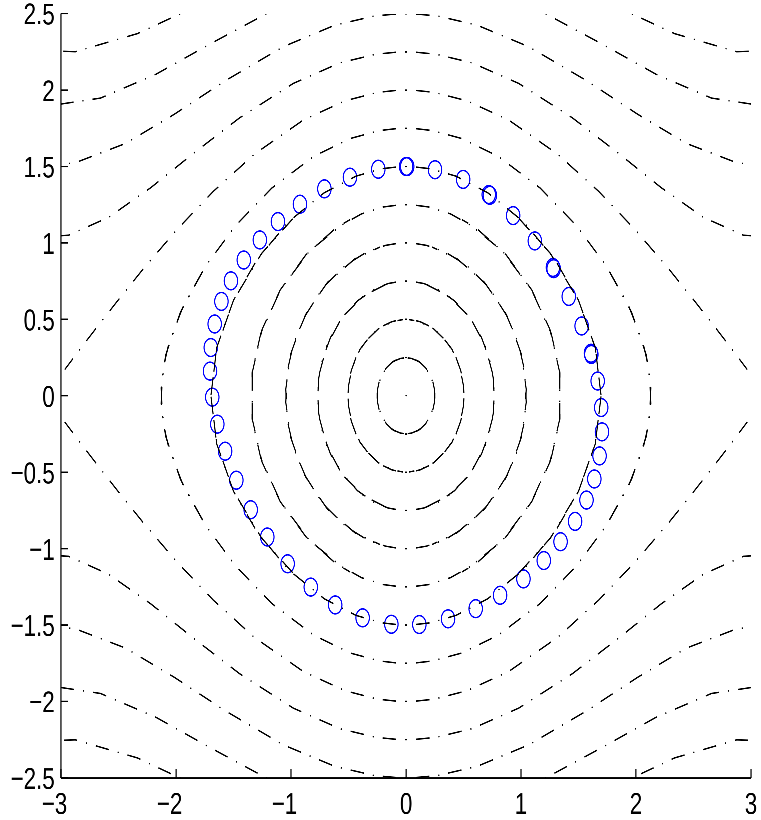
$h = 0.5$, 50 steps

SE1



SE1$_{\text{EF}}$

$\omega = 1$



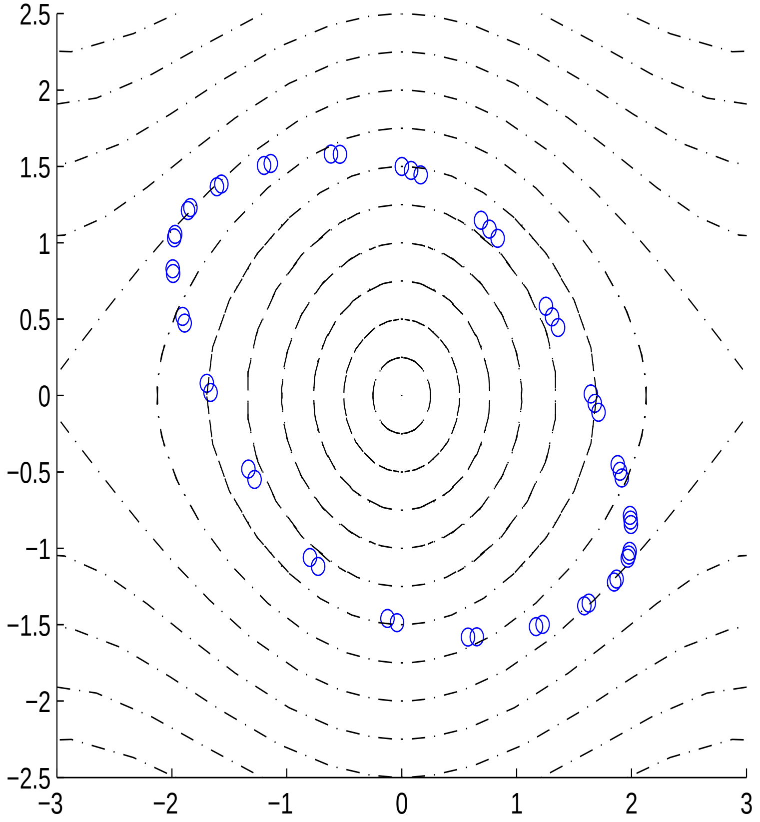
The pendulum

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

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

SE1_{EF}

$\omega = 1.4$



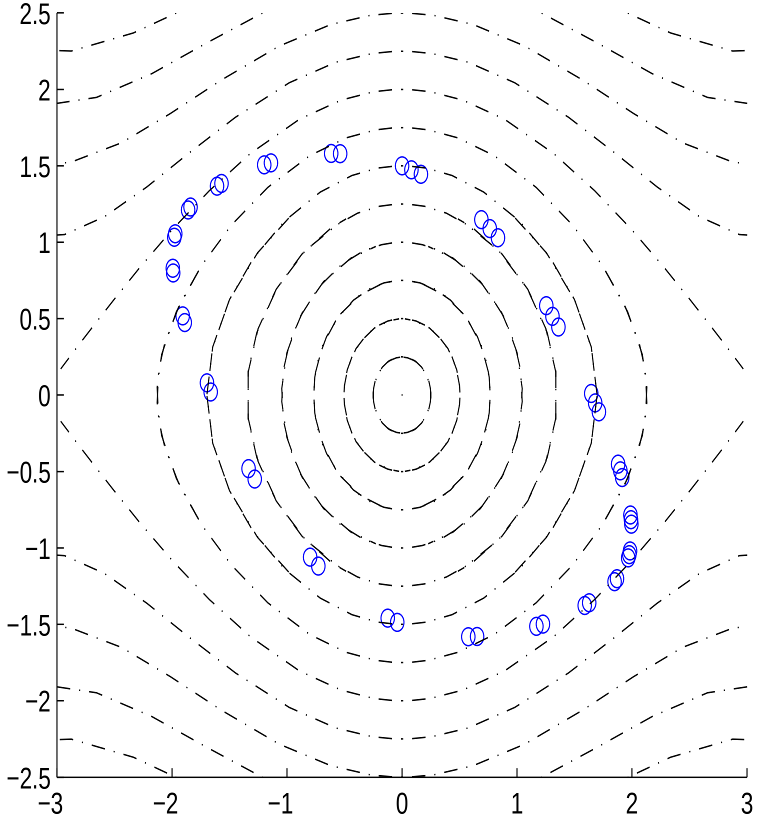
The pendulum

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

$h = 0.5$, 50 steps

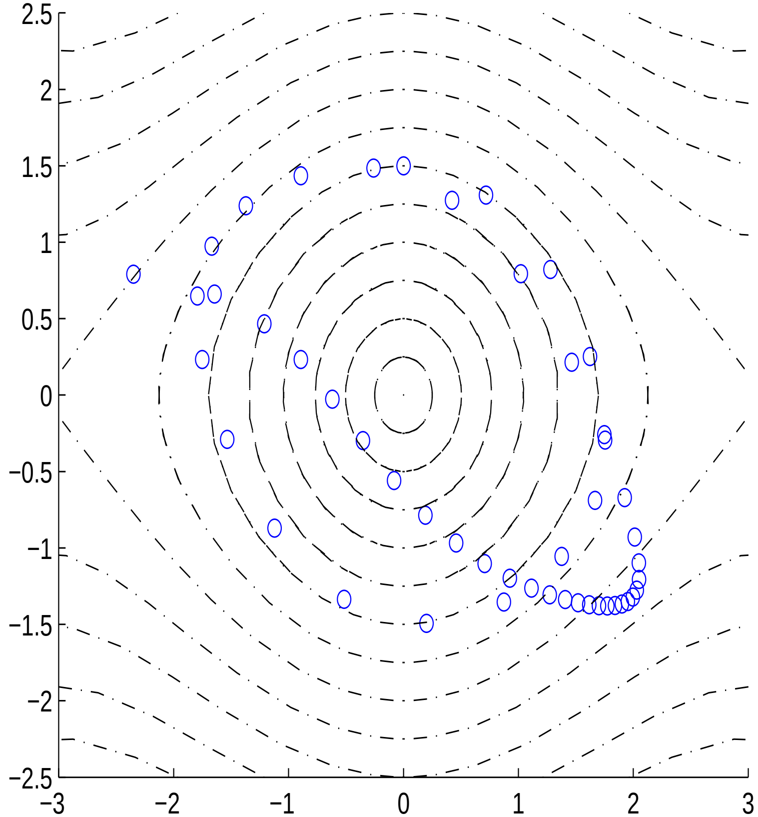
SE1$_{\text{EF}}$

$\omega = 1.4$



SE1$_{\text{EF}}$

$\omega_n = 1 + n/50$



The Störmer-Verlet method

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

Example : ω must be held constant

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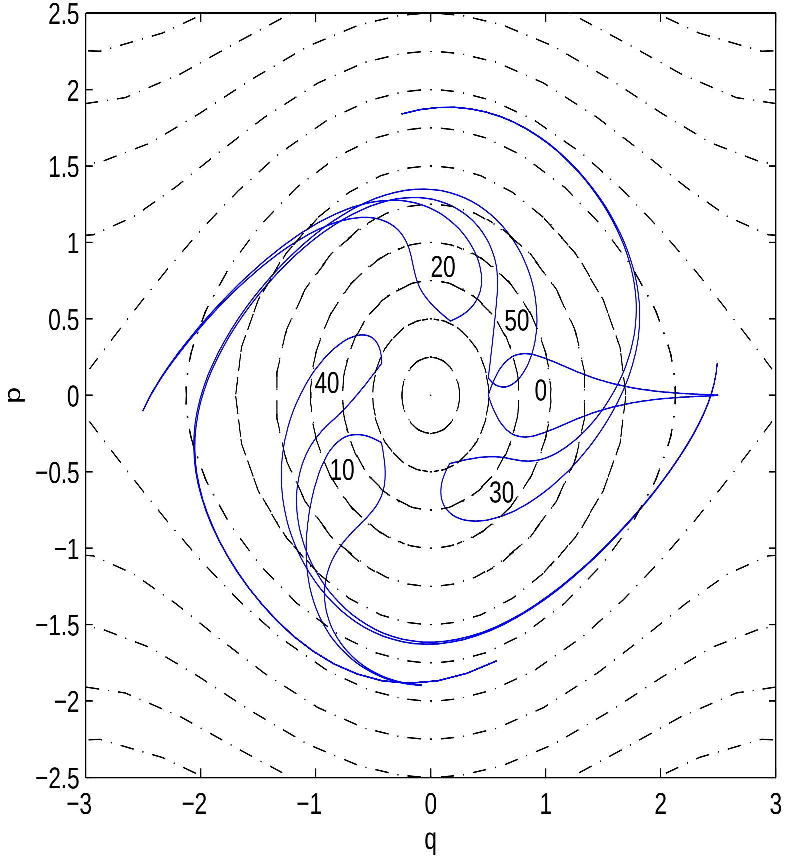
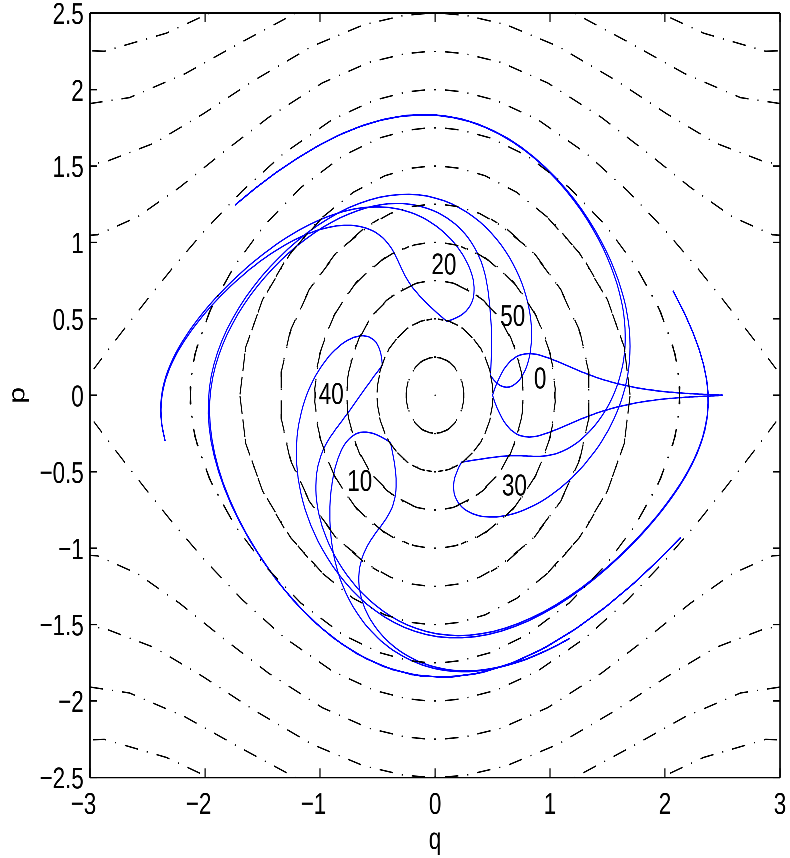
SE1



SE1_{EF}

$\omega = 1$



The pendulum : symplecticity

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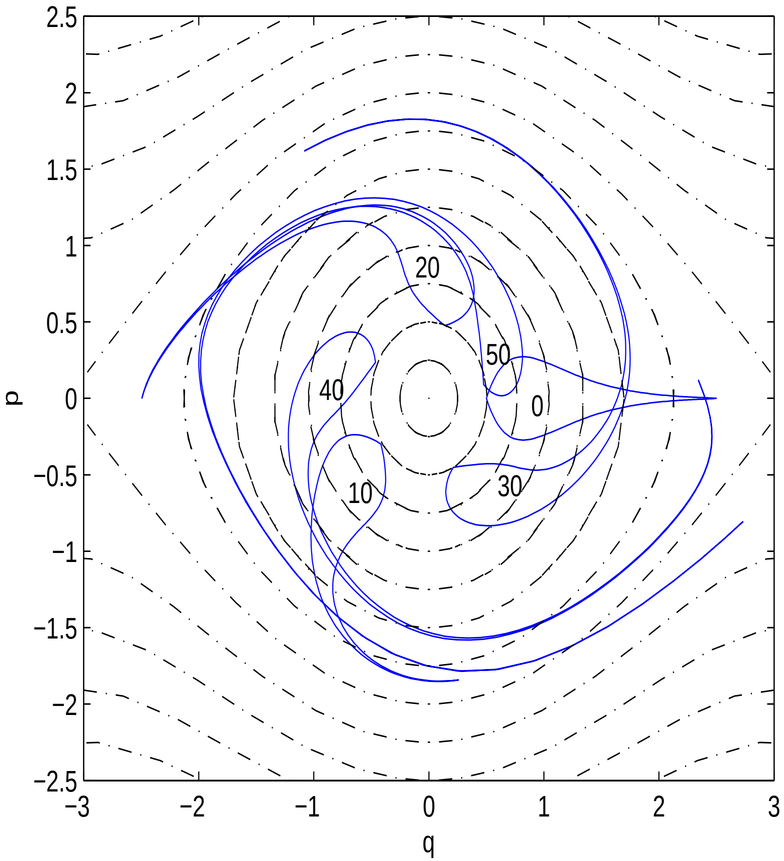
SE1$_{\text{EF}}$ $\qquad \omega_n = 1 + n/50$



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 ?

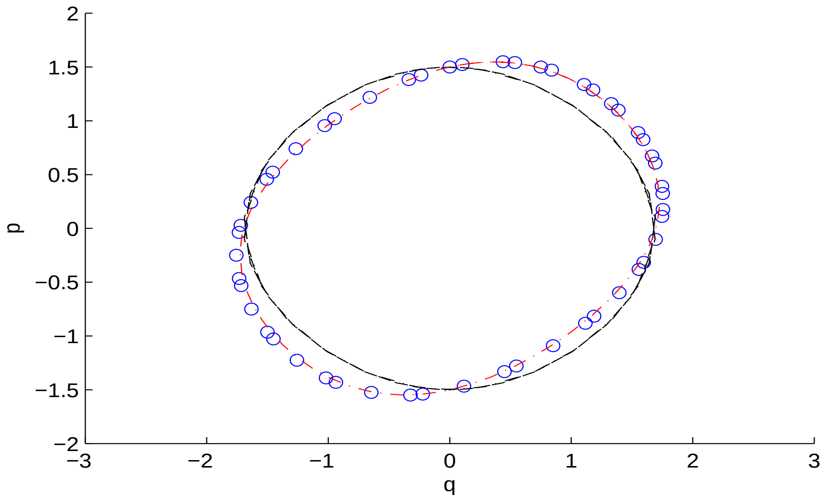
- study of modified equation : backward error analysis
- study of error in H

The pendulum : modified eqn.

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

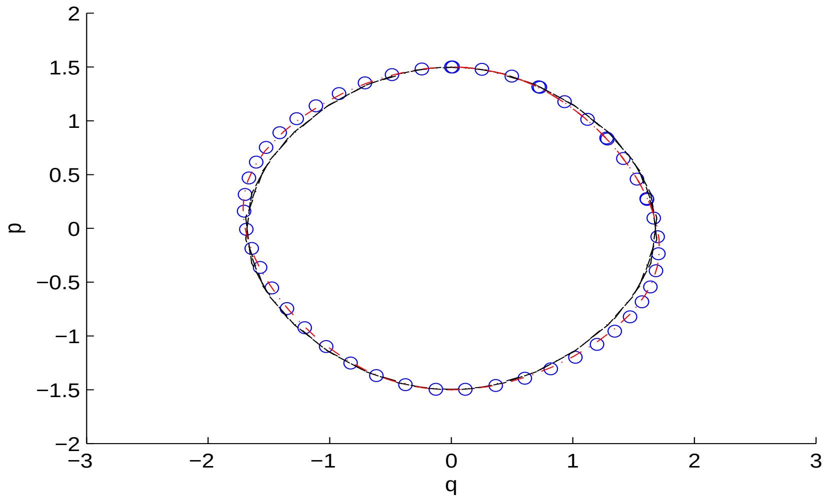
$h = 0.25$, 50 steps

SE1



SE1$_{\mathrm{EF}}$

$\omega = 1$



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

The pendulum : error in H

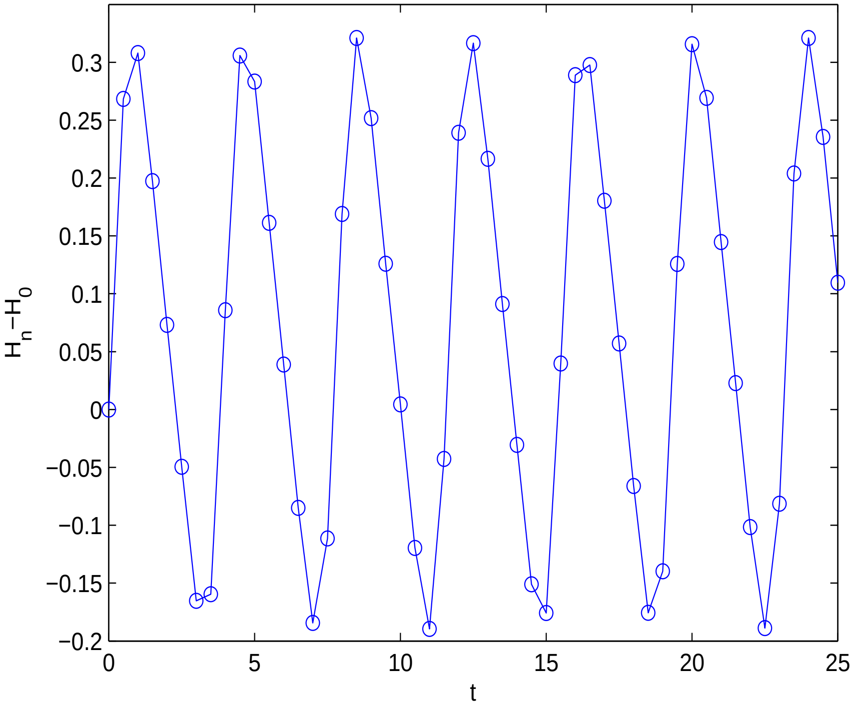
$$\ddot{q} = -\sin q, \qquad q(0) = 0, \quad \dot{q}(0) = 1.5$$

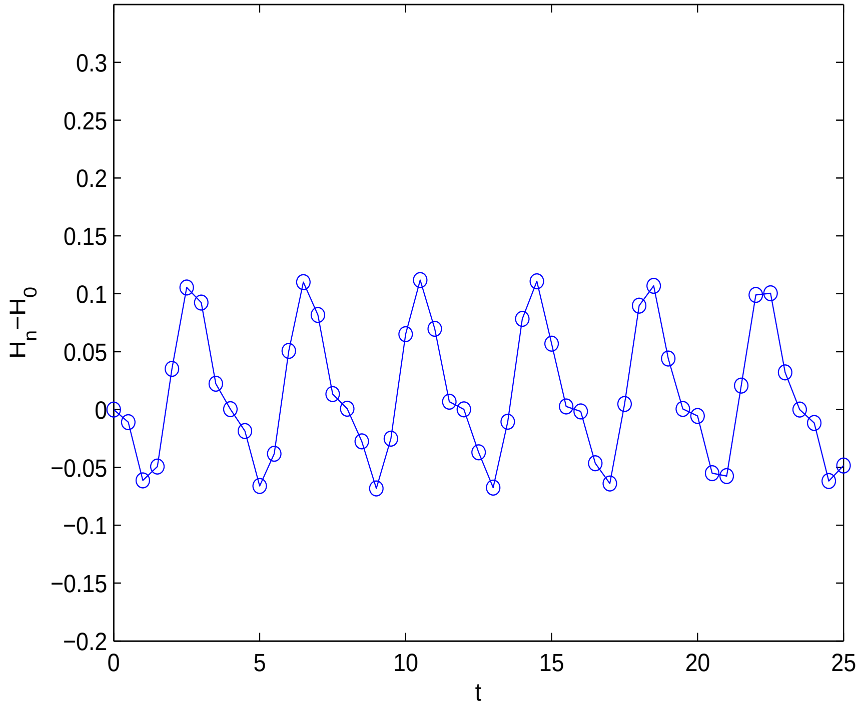
$h = 0.5$, 50 steps

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

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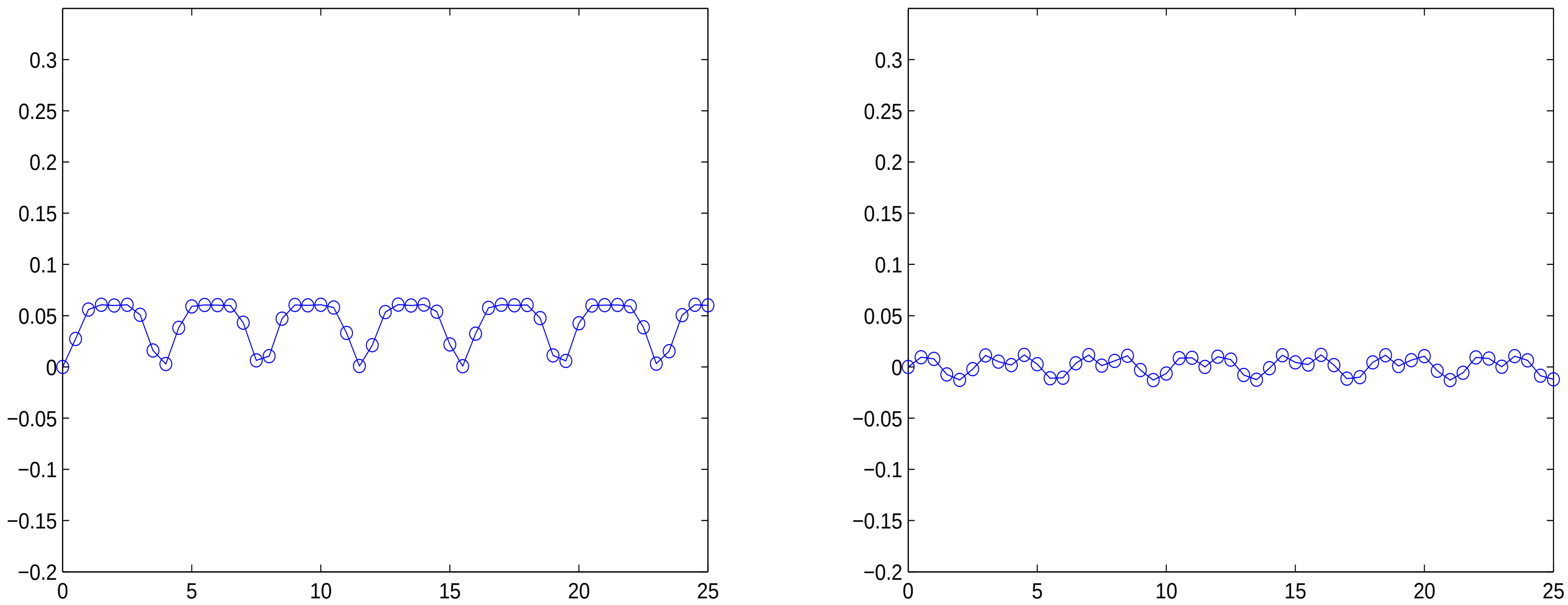

$$H_{n+1} = H_n + \frac{1}{12} \sin q_n \, p_n \left(3 \left(\omega^2 - \cos q_n\right) - p_n^2\right) \, h^3 + \mathcal{O}(h^4)$$

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.