Intégration de Simpson et schéma symplectique du quatrième ordre

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IRCAM, Paris (France)

21 novembre 2024

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preliminaries : Newmark scheme (1959)

second order dynamical system $M \frac{d^2 q}{dt^2} + C \frac{dq}{dt} + K\, q(t) = f(t)$

implicit scheme parameterized by γ and β:

see the book of Géradin and Rixen (2015)

$$\left(\frac{dq}{dt}\right)_{j+1} = \left(\frac{dq}{dt}\right)_j + h\left[(1-\gamma)\left(\frac{d^2 q}{dt^2}\right)_j + \gamma\left(\frac{d^2 q}{dt^2}\right)_{j+1}\right]$$

$$q_{j+1} = q_j + h\left(\frac{dq}{dt}\right)_j + h^2\left[\left(\frac{1}{2}-\beta\right)\left(\frac{d^2 q}{dt^2}\right)_j + \beta\left(\frac{d^2 q}{dt^2}\right)_{j+1}\right]$$

take $C = 0$, $f(t) = 0$

introduce the momentum $p \equiv M \frac{dq}{dt}$: $\frac{dp}{dt} + K\, q(t) = 0$

special case $\gamma = \frac{1}{2}$, and $\beta = \frac{1}{4}$:

$$p_{j+1} = p_j + \frac{h}{2}(-K)(q_{j+1} + q_j)$$

$$\begin{aligned} M(q_{j+1} - q_j) &= h\, p_j - \frac{h^2}{4} K (q_{j+1} + q_j) \\ &= h\, p_j + \frac{h}{2}(p_{j+1} - p_j) = \frac{h}{2}(p_{j+1} + p_j) \end{aligned}$$

Newmark scheme for a linear oscillator :

$$\frac{p_{j+1} - p_j}{h} + \frac{1}{2} K (q_{j+1} + q_j) = 0, \quad M \frac{q_{j+1} - q_j}{h} - \frac{1}{2}(p_{j+1} + p_j) = 0$$

outline

principle of least action

discrete symplecticity

$\mathbf{P_2}$ interpolation and Simpson quadrature

test for a nonlinear scalar case

two by two system: coupled linear pendula

system of dimension 3: top (preliminary result)

conclusion

annex: nonlinear pendulum

principle of least action

starting point for establishing evolution equations

action $S_c = \int_0^T L\big(\frac{\mathrm{d}q}{\mathrm{d}t},\, q(t)\big)\, \mathrm{d}t,$ state $q(t)$: unknown function

variation of the action in an infinitesimal displacement $\delta q(t)$

$$\delta S_c = \Big[\big(\frac{\partial L}{\partial \dot q}\big)\, \delta q(t)\Big]_0^T + \int_0^T \Big[\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\big(\frac{\partial L}{\partial \dot q}\big)\Big]\, \delta q(t)\, \mathrm{d}t$$

Euler-Lagrange equations $\frac{\mathrm{d}}{\mathrm{d}t}\big(\frac{\partial L}{\partial \dot q}\big) = \frac{\partial L}{\partial q}$

classical Lagrangian $L\big(\frac{\mathrm{d}q}{\mathrm{d}t},\, q\big) = \frac{m}{2}\,\big(\frac{\mathrm{d}q}{\mathrm{d}t}\big)^2 - V(q)$

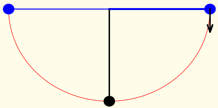
momentum $p \equiv \frac{\partial L}{\partial \dot q}$

Hamiltonian

$$H(p,\, q) \equiv p\, \frac{\mathrm{d}q}{\mathrm{d}t} - L\big(\frac{\mathrm{d}q}{\mathrm{d}t},\, q(t)\big) = \frac{p^2}{2m} + V(q)$$

Hamilton equations

$$\frac{\mathrm{d}p}{\mathrm{d}t} + \frac{\partial H}{\partial q} = 0, \quad \frac{\mathrm{d}q}{\mathrm{d}t} - \frac{\partial H}{\partial p} = 0$$



anharmonic potential
$V(q) = m\,\omega^2\,(1 - \cos q)$
$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \omega^2 \sin q = 0$

flow $\Phi :\ (p,\, q)(t = 0) \longmapsto (p,\, q)(t)$

Liouville theorem: the volume is conserved in the phase space

discrete principle of least action

split the interval $[0,\ T]$ into N elements, $h = \frac{T}{N}$, $q_j \simeq q(j\,h)$

discrete action $\quad S_d = \sum_{j=1}^{N-1} L_d(q_j,\ q_{j+1})$

discrete Lagrangian $L_d(q_\ell,\ q_r) \simeq \int_t^{t+h} \big[\frac{m}{2} \big(\frac{\mathrm{d}q}{\mathrm{d}t}\big)^2 - V(q) \big]\, \mathrm{d}t$

$\mathbf{P_1}$ internal interpolation between $q_\ell \simeq q(t)$ and $q_r \simeq q(t+h)$

centered finite difference approximation $\quad \frac{\mathrm{d}q}{\mathrm{d}t} \simeq \frac{q_r - q_\ell}{h}$

midpoint quadrature formula $\quad \int_t^{t+h} V\big(q(t)\big)\, \mathrm{d}t \simeq h\, V\big(\frac{q_\ell + q_r}{2}\big)$

$L_d(q_\ell,\ q_r) = \frac{m\,h}{2} \big(\frac{q_r - q_\ell}{h}\big)^2 - h\, V\big(\frac{q_\ell + q_r}{2}\big)$

discrete Euler Lagrange equation $\quad \frac{\partial L_d}{\partial q_r}(q_{j-1},\ q_j) + \frac{\partial L_d}{\partial q_\ell}(q_j,\ q_{j+1}) = 0$

the resulting scheme is the Newmark implicit scheme (1959)

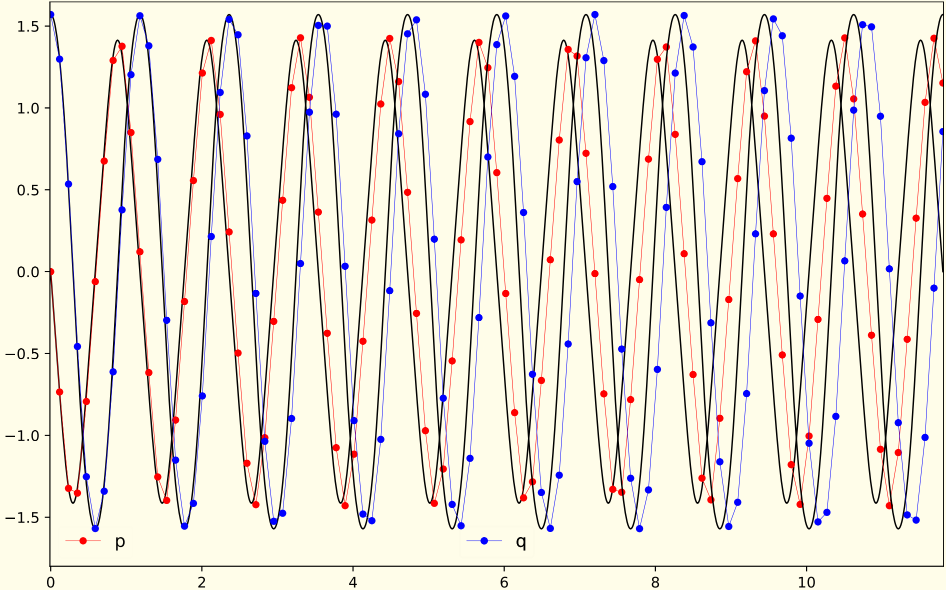
discrete moment $\quad p_r \equiv \frac{\partial L_d}{\partial q_r}$

discrete Hamilton equations

$$\frac{p_{j+1} - p_j}{h} + \frac{\partial V}{\partial q}\Big(\frac{q_j + q_{j+1}}{2}\Big) = 0, \qquad \frac{q_{j+1} - q_j}{h} - \frac{1}{2\,m}\,(p_{j+1} + p_j) = 0$$

Sanz-Serna (1992), Wendlandt, Marsden (1997), Hairer, Lubich, Wanner (2006)

anharmonic oscillator, 10 periods, 10 points per period



second order accurate Newmark scheme

discrete symplecticity

Proposition 1 [Sanz-Serna (1992)]

regular transformation $P = P(p,\, q),\;\; Q = Q(p,\, q)$

symplectic transformation: $\mathrm{d}P \wedge \mathrm{d}Q = \mathrm{d}p \wedge \mathrm{d}q$

Jacobian matrix $\alpha \equiv \frac{\partial(P,Q)}{\partial(p,q)} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$,

"imaginary" matrix $J = \begin{pmatrix} 0 & \mathrm{I} \\ -\mathrm{I} & 0 \end{pmatrix}$

classical symplecticity condition: $\alpha^{\mathrm{t}}\, J\, \alpha = J$

that can be written

(i) $a^{\mathrm{t}} c$ and $b^{\mathrm{t}} d$ are symmetric: $a^{\mathrm{t}} c = c^{\mathrm{t}} a,\;\; b^{\mathrm{t}} d = d^{\mathrm{t}} b$

(ii) $a^{\mathrm{t}} d - b^{\mathrm{t}} c$ is the identity matrix: $a^{\mathrm{t}} d - c^{\mathrm{t}} b = \mathrm{I}$.

discrete symplecticity *(ii)*

Proof of Proposition 1

$$\mathrm{d}P_i = a_i^j \, \mathrm{d}p_j + b_{ij} \, \mathrm{d}q^j , \qquad \mathrm{d}Q^i = c^{i\ell} \, \mathrm{d}p_\ell + d_\ell^i \, \mathrm{d}q^\ell$$

$$\mathrm{d}P \wedge \mathrm{d}Q = (a_i^j \, \mathrm{d}p_j + b_{ij} \, \mathrm{d}q^j) \wedge (c^{i\ell} \, \mathrm{d}p_\ell + d_\ell^i \, \mathrm{d}q^\ell)$$

$$= a_i^j \, c^{i\ell} \, \mathrm{d}p_j \wedge \mathrm{d}p_\ell + b_{ij} \, d_\ell^i \, \mathrm{d}q^j \wedge \mathrm{d}q^\ell + a_i^j \, d_\ell^i \, \mathrm{d}p_j \wedge \mathrm{d}q^\ell + b_{ij} \, c^{i\ell} \, \mathrm{d}q^j \wedge \mathrm{d}p_\ell$$

$$= (a^{\rm t} c)^{j\ell} \, \mathrm{d}p_j \wedge \mathrm{d}p_\ell + (b^{\rm t} d)_{j\ell} \, \mathrm{d}q^j \wedge \mathrm{d}q^\ell + \big[(a^{\rm t} d)_\ell^j - (c^{\rm t} b)_\ell^j \big] \, \mathrm{d}p_j \wedge \mathrm{d}q^\ell$$

$\equiv \mathrm{d}p_j \wedge \mathrm{d}q^j$ if and only if

(i) $a^{\rm t} c$ and $b^{\rm t} d$ are symmetric: $a^{\rm t} c = c^{\rm t} a, \; b^{\rm t} d = d^{\rm t} b$

(ii) $a^{\rm t} d - b^{\rm t} c$ is the identity matrix: $a^{\rm t} d - c^{\rm t} b = \mathrm{I}$

then

$$\alpha^{\rm t} J \, \alpha = \begin{pmatrix} a^{\rm t} & c^{\rm t} \\ b^{\rm t} & d^{\rm t} \end{pmatrix} \begin{pmatrix} 0 & \mathrm{I} \\ -\mathrm{I} & 0 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a^{\rm t} & c^{\rm t} \\ b^{\rm t} & d^{\rm t} \end{pmatrix} \begin{pmatrix} c & d \\ -a & -b \end{pmatrix}$$

$$= \begin{pmatrix} a^{\rm t} c - c^{\rm t} a & a^{\rm t} d - c^{\rm t} b \\ b^{\rm t} c - d^{\rm t} a & b^{\rm t} d - d^{\rm t} b \end{pmatrix} = \begin{pmatrix} 0 & \mathrm{I} \\ -\mathrm{I} & 0 \end{pmatrix} = J \qquad \square$$

discrete symplecticity *(iii)*

Proposition 2 [Lewis & Simo (1995), Wendlandt & Marsden (1997)]
A numerical scheme obtained with a discrete set of Euler-Lagrange equations is symplectic.

discrete action $S_d = .. + L_d(q_{j-1},\, q_j) + L_d(q_j,\, q_{j+1}) + ...$

discrete Euler-Lagrange equations: $\frac{\partial L_d}{\partial q_r}(q_{j-1},\, q_j) + \frac{\partial L_d}{\partial q_\ell}(q_j,\, q_{j+1}) = 0$

right momentum $p_r = \frac{\partial L_d}{\partial q_r}(q_\ell,\, q_r)$ or $p_j = \frac{\partial L_d}{\partial q_r}(q_{j-1},\, q_j)$

discrete Euler-Lagrange equations: $p_j + \frac{\partial L_d}{\partial q_\ell}(q_j,\, q_{j+1}) = 0$

discrete Hamiltonian $H_d = p_r\, q_r - L_d(q_\ell,\, q_r)$

then $\mathrm{d}H_d = \mathrm{d}p_r\, q_r + p_r\, \mathrm{d}q_r - \frac{\partial L_d}{\partial q_\ell}\, \mathrm{d}q_\ell - p_r\, \mathrm{d}q_r = -\frac{\partial L_d}{\partial q_\ell}\, \mathrm{d}q_\ell + \mathrm{d}p_r\, q_r$

$$H_d = H_d(q_\ell,\, p_r), \quad \frac{\partial H_d}{\partial q_\ell}(q_\ell,\, p_r) = -\frac{\partial L_d}{\partial q_\ell}(q_\ell,\, q_r), \quad \frac{\partial H_d}{\partial p_r}(q_\ell,\, p_r) = q_r$$

discrete Euler-Lagrange becomes discrete (implicit) Hamilton

$$p_j - \frac{\partial H_d}{\partial q_\ell}(q_j,\, p_{j+1}) = 0, \quad q_{j+1} = \frac{\partial H_d}{\partial p_r}(q_j,\, p_{j+1})$$

Jacobian matrix $\alpha = \begin{pmatrix} \frac{\partial p_{j+1}}{\partial p_j} & \frac{\partial p_{j+1}}{\partial q_j} \\ \frac{\partial q_{j+1}}{\partial p_j} & \frac{\partial q_{j+1}}{\partial q_j} \end{pmatrix}$; $\alpha^{\mathrm{t}}\, J\, \alpha = J$?

discrete symplecticity *(iv)*

differentiate the discrete Hamilton equations

$$\mathrm{d}p_j - \frac{\partial^2 H_d}{\partial q_\ell^2}\,\mathrm{d}q_j - \frac{\partial^2 H_d}{\partial q_\ell\,\partial p_\ell}\,\mathrm{d}p_{j+1} = 0$$

$$\mathrm{d}q_{j+1} = \frac{\partial^2 H_d}{\partial p_r\,\partial q_\ell}\,\mathrm{d}q_j + \frac{\partial^2 H_d}{\partial p_r^2}\,\mathrm{d}p_{j+1}$$

the Hessian matrix is symmetric

$H''_q \equiv \frac{\partial^2 H_d}{\partial q_\ell^2}$, $H''_p = \frac{\partial^2 H_d}{\partial p_r^2}$, $\gamma \equiv \frac{\partial^2 H_d}{\partial q_\ell\,\partial p_\ell}$ are symmetric matrices

hypothesis: the matrix γ is invertible. Then

$$\mathrm{d}p_{j+1} = \gamma^{-1}\,\mathrm{d}p_j - \gamma^{-1}\,H''_q\,\mathrm{d}q_j$$

$$-H''_p\,\mathrm{d}p_{j+1} + \mathrm{d}q_{j+1} = \gamma\,\mathrm{d}q_j$$

id est $\begin{pmatrix} \mathrm{I} & 0 \\ -H''_p & \mathrm{I} \end{pmatrix} \begin{pmatrix} \mathrm{d}p_{j+1} \\ \mathrm{d}q_{j+1} \end{pmatrix} = \begin{pmatrix} \gamma^{-1} & -\gamma^{-1}\,H''_q \\ 0 & \gamma \end{pmatrix} \begin{pmatrix} \mathrm{d}p_j \\ \mathrm{d}q_j \end{pmatrix}$

with $\begin{pmatrix} \mathrm{d}p_{j+1} \\ \mathrm{d}q_{j+1} \end{pmatrix} \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \mathrm{d}p_j \\ \mathrm{d}q_j \end{pmatrix} \equiv \alpha \begin{pmatrix} \mathrm{d}p_j \\ \mathrm{d}q_j \end{pmatrix}$, we have

we have $\begin{pmatrix} \mathrm{I} & 0 \\ -H''_p & \mathrm{I} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \gamma^{-1} & -\gamma^{-1}\,H''_q \\ 0 & \gamma \end{pmatrix}$

discrete symplecticity *(v)*

$$\begin{pmatrix} \mathrm{I} & 0 \\ -H''_p & \mathrm{I} \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \gamma^{-1} & -\gamma^{-1} \, H''_q \\ 0 & \gamma \end{pmatrix}$$

4 relations

$$\begin{aligned} a &= \gamma^{-1} \\ -H''_p \, a + c &= 0 \\ b &= -\gamma^{-1} \, H''_q \\ -H''_p \, b + d &= \gamma \end{aligned}$$

3 conditions to satisfy $\quad a^{\mathrm{t}} c = c^{\mathrm{t}} a, \;\; b^{\mathrm{t}} d = d^{\mathrm{t}} b, \;\; a^{\mathrm{t}} d - c^{\mathrm{t}} b = \mathrm{I}$

(i) $\quad c = H''_p \, a$ then $a^{\mathrm{t}} c = a^{\mathrm{t}} \, H''_p \, a$ is symmetric

(ii) $\quad d = \gamma + H''_p \, b$

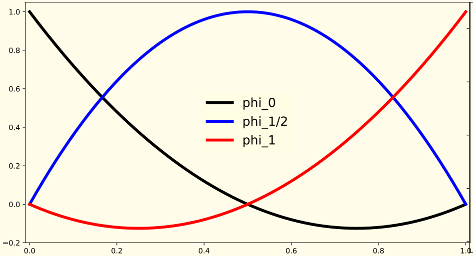
$d^{\mathrm{t}} = \gamma + b^{\mathrm{t}} \, H''_p$ because γ and H''_p are symmetric

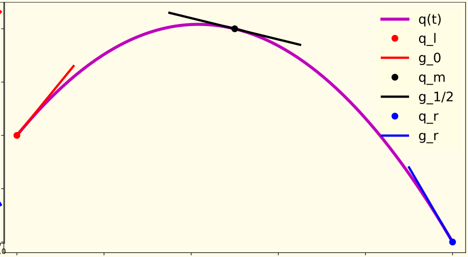
$d^{\mathrm{t}} b = \gamma \, b + b^{\mathrm{t}} \, H''_p \, b = -H''_q + b^{\mathrm{t}} \, H''_p \, b$ symmetric

(iii) $\quad a^{\mathrm{t}} d - c^{\mathrm{t}} b = a^{\mathrm{t}} \, (\gamma + H''_p \, b) - a^{\mathrm{t}} \, H''_p \, b$

$= a^{\mathrm{t}} \, \gamma = \mathrm{I}$ because $a = \gamma^{-1}$. $\square$

finite elements with quadratic interpolation





basis function of the $\mathbf{P_2}$ finite element

$$\varphi_0(\theta) = (1-\theta)\,(1-2\,\theta)\,,\ \ \varphi_{1/2}(\theta) = 4\,\theta\,(1-\theta)\,,\ \ \varphi_1(\theta) = \theta\,(2\,\theta-1)$$

$$0 \leq \theta \leq 1$$

interpolating polynomial function

$$q(t) = q_\ell\,\varphi_0(\theta) + q_m\,\varphi_{1/2}(\theta) + q_r\,\varphi_1(\theta)$$

discrete derivatives

$$g_\ell = \frac{1}{h}\,(-3\,q_\ell + 4\,q_m - q_r),\ \ g_m = \frac{q_r - q_\ell}{h},\ \ g_r = \frac{1}{h}\,(q_\ell - 4\,q_m + 3\,q_r)$$

C. William Gear (1971)

Simpson's quadrature for a discrete Lagrangian

numerical integration on the interval $[0, 1]$

midpoint formula: $\int_0^1 \psi(\theta)\, \mathrm{d}\theta \simeq \psi(\frac{1}{2})$

exact for a polynomial ψ of degree ≤ 1

Thomas Simpson (1710-1761) quadrature:

$$\int_0^1 \psi(\theta)\, \mathrm{d}\theta \simeq \frac{1}{6}\Big[\psi(0) + 4\,\psi\Big(\frac{1}{2}\Big) + \psi(1)\Big]$$

exact for any polynomial ψ of degree ≤ 3

discrete Lagrangian with the Simpson quadrature formula

$$L_h(q_\ell,\, q_m,\, q_r) \simeq \int_t^{t+h} \Big[\frac{1}{2}\, M \,(\frac{\mathrm{d}q}{\mathrm{d}t})^2 - V(q)\Big]\, \mathrm{d}t$$

$$L_h(q_\ell,\, q_m,\, q_r) = \frac{h}{12}\, M \,({g_\ell}^2 + 4\, g_m^2 + {g_r}^2) - \frac{h}{6}\,(V(q_\ell) + 4\, V(q_m) + V(q_r))$$

with

$$g_\ell = \frac{1}{h}\,(-3\, q_\ell + 4\, q_m - q_r),\quad g_m = \frac{q_r - q_\ell}{h},\quad g_r = \frac{1}{h}\,(q_\ell - 4\, q_m + 3\, q_r)$$

discrete Euler-Lagrange equations: middle point

discrete action $\Sigma_d = \sum_{j=1}^{N-1} L_h(q_j,\, q_{j+1/2},\, q_{j+1})$

Maupertuis's least-action principle $\delta\Sigma_d = 0$

for arbitrary variations δq_j and $\delta q_{j+1/2}$

$$L_h(q_\ell,\, q_m,\, q_r) = \frac{h}{12}\, M\big({g_\ell}^2 + 4\, g_m^2 + {g_r}^2\big) - \frac{h}{6}\, \big(V(q_\ell) + 4\, V(q_m) + V(q_r)\big)$$

Euler-Lagrange equations first established for an arbitrary variation of the internal degree of freedom $\delta q_{j+1/2}$: $\frac{\partial L_S}{\partial q_m} = 0$

we have $\frac{\partial g_\ell}{\partial q_m} = \frac{4}{h},\ \frac{\partial g_m}{\partial q_m} = 0,\ \frac{\partial g_r}{\partial q_m} = -\frac{4}{h},\ V'_m \equiv \frac{\partial V}{\partial q}(q_m)$

$$\frac{\partial L_S}{\partial q_m} = \frac{h}{6}\, M\big(g_\ell\, \frac{4}{h} + g_\ell\, \frac{4}{h}\big) - \frac{2}{3}\, h\, V'_m = \frac{16}{3h}\, M\Big[q_m - \frac{1}{2}\, (q_\ell + q_r) - \frac{h^2}{8\, m}\, V'_m\Big]$$

$q_m - \frac{h^2}{8}\, M^{-1}\, \frac{\partial V}{\partial q}(q_m) = \frac{1}{2}\, (q_\ell + q_r)$: defines implicitly the value q_m as a function of the extremities q_ℓ and q_r:

$$\frac{4}{h^2}\, M\, (q_\ell - 2\, q_m + q_r) + \frac{\partial V}{\partial q}(q_m) = 0$$

consistent with the differential equation $M\, \frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \frac{\partial V}{\partial q} = 0$

then the numerical scheme is symplectic !

discrete Euler-Lagrange equations: extremities

discrete action

$$\Sigma_d = \cdots + L_h(q_{j-1},\, q_{j-1/2},\, q_j) + L_h(q_j,\, q_{j+1/2},\, q_{j+1}) + \ldots .$$

variation relative to q_j equal to zero

discrete Euler-Lagrange equations:

$$\frac{\partial L_S}{\partial q_r}(q_{j-1},\, q_{j-1/2},\, q_j) + \frac{\partial L_S}{\partial q_\ell}(q_j,\, q_{j+1/2},\, q_{j+1}) = 0$$

after some lines of elementary calculus

$$\frac{1}{h^2}\left(q_{j-1} - 2\,q_j + q_{j+1}\right) + \frac{1}{3}\,M^{-1}\left(V'_{j-1/2} + V'_j + V'_{j+1/2}\right) = 0$$

consistent with the differential equation $M\,\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \frac{\partial V}{\partial q} = 0$

discrete momentum

right momentum $p_r \equiv \dfrac{\partial L_S}{\partial q_r}$

$$p_r = \tfrac{h}{6}\, M \left[g_\ell \left(-\tfrac{1}{h} \right) + 4\, g_m \left(\tfrac{1}{h} \right) + g_r \left(\tfrac{3}{h} \right) \right] - \tfrac{h}{6}\, V'_r$$

$$= \tfrac{1}{6} \left[\tfrac{2}{h}\, M \left(q_\ell - 8\, q_m + 7\, q_r \right) - h\, V'_r \right]$$

$$\text{with } q_m = \tfrac{1}{2} (q_\ell + q_r) + \tfrac{h^2}{8}\, M^{-1} \tfrac{\partial V}{\partial q}(q_m)$$

$$p_r = \tfrac{1}{h}\, M \left(q_r - q_\ell \right) - \tfrac{h}{6} \left(2\, V'_m + V'_r \right)$$

with space indices: $p_{j+1} = \dfrac{1}{h}\, M \left(q_{j+1} - q_j \right) - \dfrac{h}{6} \left(2\, V'_{j+1/2} + V'_{j+1} \right)$

similarly, $p_j = \tfrac{1}{h}\, M \left(q_j - q_{j-1} \right) - \tfrac{h}{6} \left(2\, V'_{j-1/2} + V'_j \right)$

taking into account the discrete Euler-Lagrange equations

$$\tfrac{1}{h^2} \left(q_{j-1} - 2\, q_j + q_{j+1} \right) + \tfrac{1}{3}\, M^{-1} \left(V'_{j-1/2} + V'_j + V'_{j+1/2} \right) = 0$$

$$p_j = \frac{1}{h}\, M \left(q_{j+1} - q_j \right) + \frac{h}{6} \left(V'_j + 2\, V'_{j+1/2} \right)$$

discrete Hamilton equations

expressions of the moments

$$p_{j+1} = \frac{1}{h} M \left(q_{j+1} - q_j \right) - \frac{h}{6} \left(2\, V'_{j+1/2} + V'_{j+1} \right)$$
$$p_j = \frac{1}{h} M \left(q_{j+1} - q_j \right) + \frac{h}{6} \left(V'_j + 2\, V'_{j+1/2} \right)$$

discrete Hamiltonian equations

$$p_{j+1} - p_j + \frac{h}{6} \left(V'_j + 4\, V'_{j+1/2} + V'_{j+1} \right) = 0$$
$$q_{j+1} - q_j - \frac{h^2}{12} M^{-1} \left(V'_{j+1} - V'_j \right) - \frac{h}{2} M^{-1} \left(p_{j+1} + p_j \right) = 0$$

discrete system to solve at each time step

$$q_{j+1/2} - \frac{h^2}{8} M^{-1} V'_{j+1/2} - \frac{1}{2} q_{j+1} = \frac{1}{2} q_j$$
$$p_{j+1} + \frac{h}{6} \left(4\, V'_{j+1/2} + V'_{j+1} \right) = p_j - \frac{h}{6} V'_j$$
$$q_{j+1} - \frac{h}{2} M^{-1} p_{j+1} - \frac{h^2}{12} M^{-1} V'_{j+1} = q_j + \frac{h}{2} M^{-1} p_j - \frac{h^2}{12} M^{-1} V'_j$$

write this nonlinear system under the form $F_S(q_{j+1/2},\, p_{j+1},\, q_{j+1}) = 0$

numerical resolution of one time step with Newton

$$F_S(q_{j+1/2},\, p_{j+1},\, q_{j+1}) = 0$$

Jacobian matrix

$$\mathrm{d}F_S(q_m,\, p,\, q) = \begin{pmatrix} \mathrm{I} - \frac{h^2}{8} M^{-1} K & 0 & -\frac{1}{2}\,\mathrm{I} \\ \frac{2}{3}\, h\, K & \mathrm{I} & \frac{h}{6}\, K \\ 0 & -\frac{h}{2} M^{-1} & \mathrm{I} - \frac{h^2}{12} M^{-1} K \end{pmatrix}$$

with $K = V''(q_m)$

inverse of the Jacobian matrix (formal calculus, scalar case)

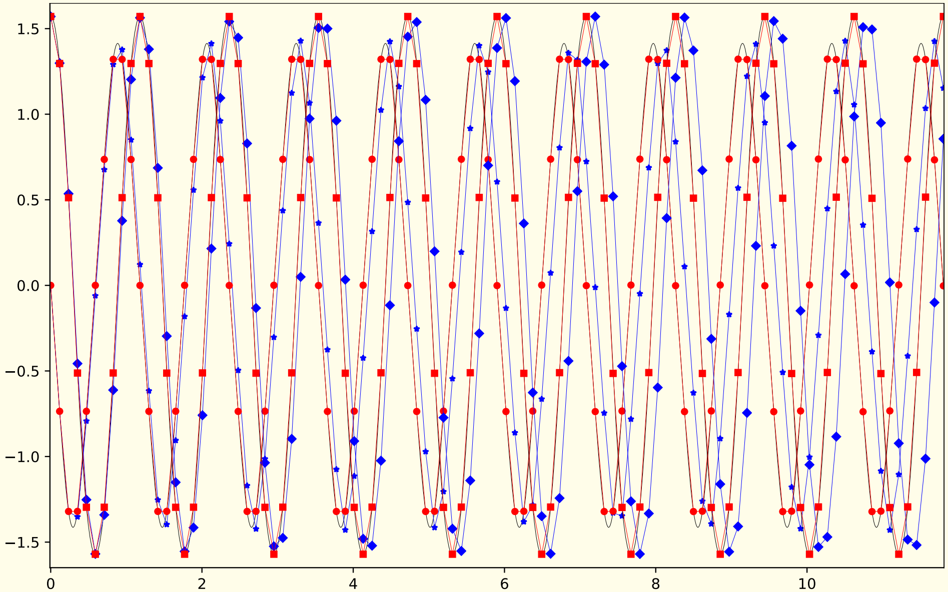
$$\mathrm{d}F_S(q_m,\, p,\, q)\big)^{-1} =$$

$$\begin{bmatrix} 1 & \frac{1}{4}\, \frac{h}{m} & \frac{1}{2} \\ -\frac{2}{3}\, m\theta + \frac{1}{18}\, hm\theta\varphi & 1 - \frac{1}{8}\, h\theta - \frac{1}{12}\, h\varphi + \frac{1}{96}\, h^2\theta\varphi & -\frac{1}{3}\, m\theta - \frac{1}{6}\, m\varphi + \frac{1}{48}\, hm\,\theta\,\varphi \\ -\frac{1}{3}\, h\,\theta & \frac{1}{2}\, \frac{h}{m} - \frac{1}{16}\, \frac{h^2\,\theta}{m} & 1 - \frac{1}{8}\, h\,\theta \end{bmatrix}$$

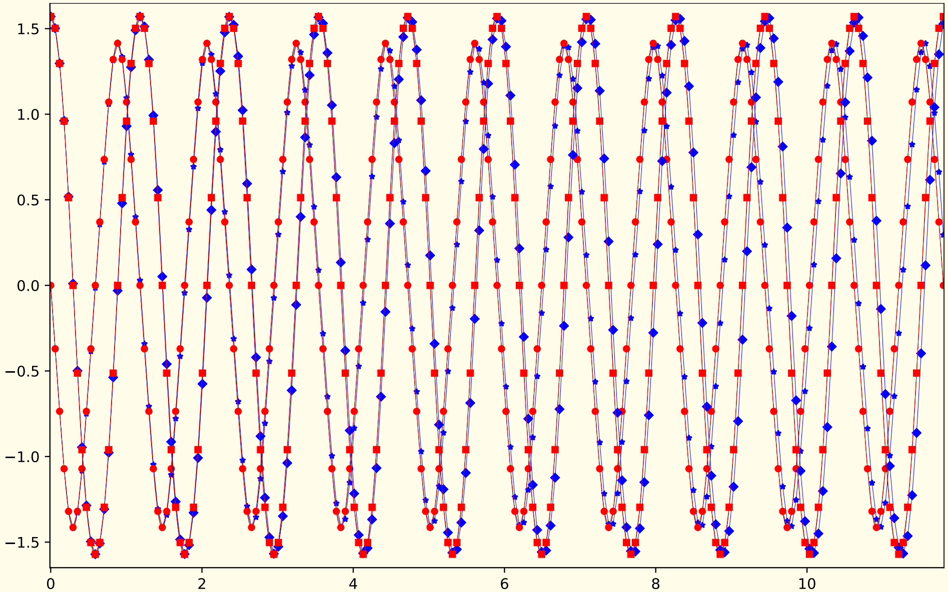
with $\theta \equiv \frac{h}{m} K$ and $\varphi \equiv \frac{h}{m} V''(q)$

Newton algorithm: machine precision convergence at the fifth iteration

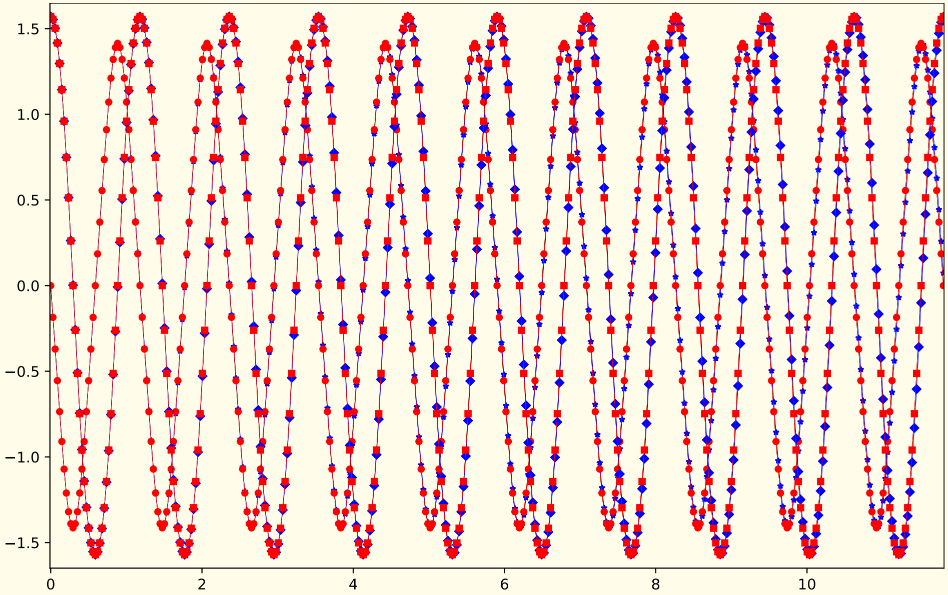
Simpson *vs* Newmark, 10 meshes per period



Simpson *vs* Newmark, 20 meshes per period



Simpson *vs* Newmark, 40 meshes per period



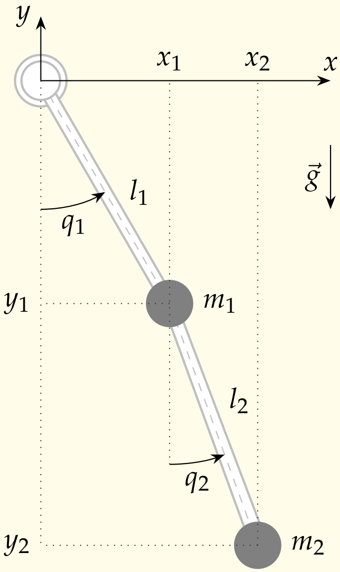
errors and order of convergence

10 periods	number of meshes	200	400	800	order
Newmark	momentum	$1.85\ 10^{0}$	$4.59\ 10^{-1}$	$1.14\ 10^{-1}$	2.01
Simpson	momentum	$1.12\ 10^{-3}$	$6.80\ 10^{-5}$	$4.20\ 10^{-6}$	4.03
Newmark	state	$3.97\ 10^{-1}$	$1.00\ 10^{-1}$	$2.51\ 10^{-2}$	1.99
Simpson	state	$2.45\ 10^{-4}$	$1.48\ 10^{-5}$	$9.16\ 10^{-7}$	4.03

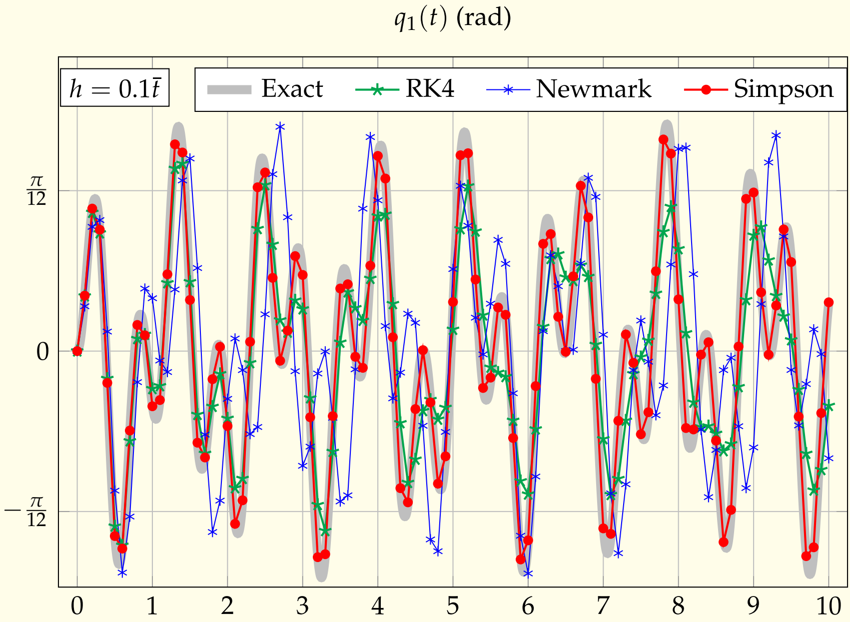
100 periods	number of meshes	2000	4000	8000	order
Newmark	momentum	$1.65\ 10^{1}$	$4.56\ 10^{0}$	$1.14\ 10^{0}$	1.92
Simpson	momentum	$1.08\ 10^{-2}$	$6.48\ 10^{-4}$	$4.01\ 10^{-5}$	4.04
Newmark	state	$2.99\ 10^{0}$	$1.01\ 10^{0}$	$2.57\ 10^{-1}$	1.77
Simpson	state	$2.43\ 10^{-3}$	$1.45\ 10^{-4}$	$8.98\ 10^{-6}$	4.04

1000 periods	number of meshes	20000	40000	80000	order
Newmark	momentum	$1.78\ 10^{1}$	$1.78\ 10^{1}$	$1.24\ 10^{1}$	0.33
Simpson	momentum	$1.08\ 10^{-1}$	$6.47\ 10^{-3}$	$4.00\ 10^{-4}$	4.04
Newmark	state	$3.14\ 10^{0}$	$3.14\ 10^{0}$	$2.26\ 10^{0}$	0.23
Simpson	state	$2.43\ 10^{-2}$	$1.46\ 10^{-3}$	$9.00\ 10^{-5}$	4.04

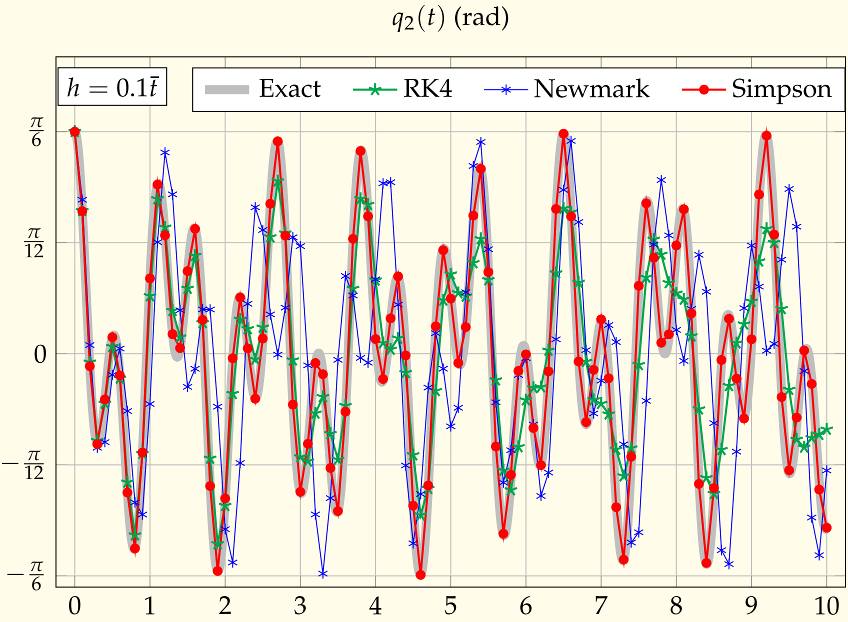
double linear pendulum



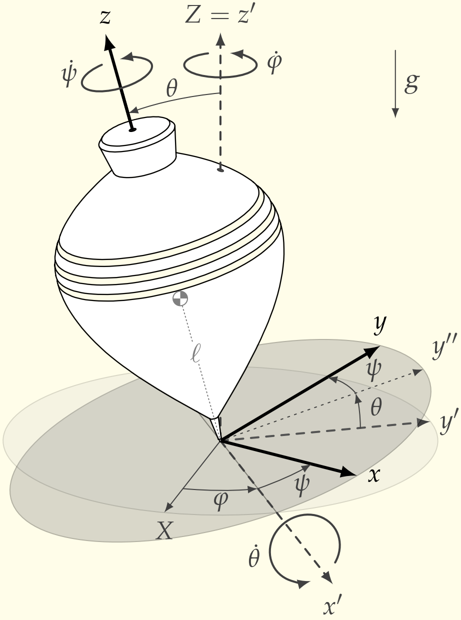
double linear pendulum: first variable



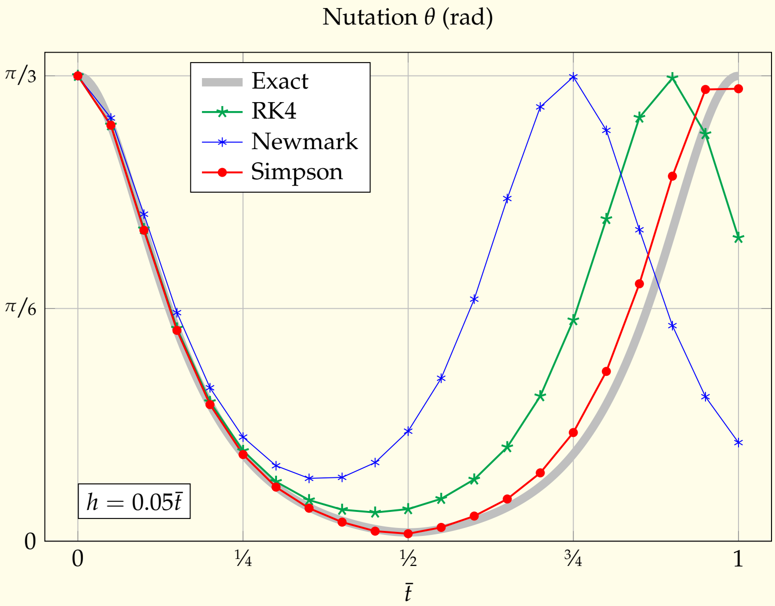
double linear pendulum: second variable



top



top: nutation



conclusion and perspectives

symplectic Simpson numerical scheme

linear and a nonlinear pendulum

fourth order accuracy

  numerically established for a nonlinear oscillator

    and a linear double pendulum

stability proven in the linear case

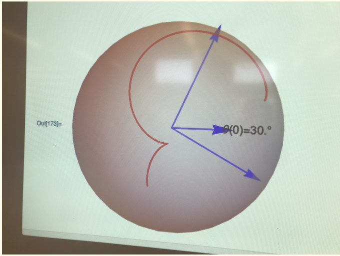
  under a natural condition $0 < \omega_{\max} \, h < 2\sqrt{2}$

system case : nonlinear test cases under study

to do:

covariant extension to mutiple dimensions

adjoint version for dynamic control



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Geometric Science of Information 2023, LNCS 14072,
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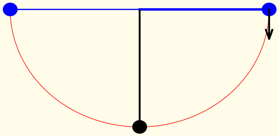
Simpson's Variational Integrator for Systems with Quadratic Lagrangians
Axioms, volume 13, article 255 (23 pages), 2024.

merci de votre attention !

annex: nonlinear pendulum [see Chenciner (2000)]

[$\theta_0 = \frac{\pi}{2}$ on the picture]



angle $\theta_0 \in (0,\, \pi)$

non linear pendulum problem

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \omega^2 \sin q = 0, \;\; q(0) = \theta_0, \;\; \frac{\mathrm{d}q}{\mathrm{d}t}(0) = 0$$

conservation of energy

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[\frac{1}{2}\Big(\frac{\mathrm{d}q}{\mathrm{d}t}\Big)^2 + \omega^2\,(1 - \cos q)\Big] = 0$$

parameter $k \equiv \sin\,\big(\frac{\theta_0}{2}\big)$ and $0 < k < 1$.

observe that $\frac{\mathrm{d}q}{\mathrm{d}t} < 0$ for small values of $t > 0$

then $\frac{\mathrm{d}q}{\mathrm{d}t} = -2\,\omega\,k\,\sqrt{1 - \frac{1}{k^2}\,\sin^2\big(\frac{q}{2}\big)} = -2\,\omega\,k\,\cos\varphi$

change of unknown $\sin\varphi = \frac{1}{k}\,\sin\big(\frac{q}{2}\big)$

then $\varphi(0) = \frac{\pi}{2}$ and $\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\omega\,\sqrt{1 - k^2\,\sin^2\varphi} = -\omega\,\cos\big(\frac{q}{2}\big)$

differential relation $\omega\,\mathrm{d}t = -\frac{\mathrm{d}\varphi}{\sqrt{1-k^2\,\sin^2\varphi}}$

nonlinear pendulum *(ii)*

incomplete elliptic integral of the first kind

$$F(a,\, m) \equiv \int_0^a \frac{\mathrm{d}\varphi}{\sqrt{1 - m \, \sin^2 \varphi}}$$

complete elliptic integral of the first kind

$$K(m) \equiv \int_0^{\pi/2} \frac{\mathrm{d}\varphi}{\sqrt{1 - m \, \sin^2 \varphi}} = F(\tfrac{\pi}{2},\, m)$$

integrate the differential relation $\omega \, \mathrm{d}t = - \frac{\mathrm{d}\varphi}{\sqrt{1 - k^2 \, \sin^2 \varphi}}$

$$\omega \, t = - \int_{\pi/2}^{\varphi} \frac{\mathrm{d}\xi}{\sqrt{1 - k^2 \, \sin^2 \xi}} = K(k^2) - F(\varphi,\, k^2)$$

after a fourth of a period T, the parameter φ changes from $\frac{\pi}{2}$ to zero: $\omega \, \frac{T}{4} = \int_0^{\pi/2} \frac{\mathrm{d}\varphi}{\sqrt{1 - k^2 \, \sin^2 \varphi}} = K(k^2)$

Jacobi amplitude $A(.,\, m)$

reciprocal function of the incomplete elliptic integral of the first kind

$F(a,\, m) = u$ is equivalent to $a = A(u,\, m)$

we have $F(\varphi,\, k^2) = K(k^2) - \omega \, t$ and $\varphi = A(K(k^2) - \omega \, t,\, k^2)$

$\sin\left(\frac{q}{2}\right) = k \, \sin\varphi, \; \frac{\mathrm{d}q}{\mathrm{d}t} = -2 \, \omega \, k \, \cos\varphi$