Un intégrateur variationnel symplectique du 6e ordre

François Dubois[*,†] and Juan Antonio Rojas-Quintero[‡]

Réunion du groupement de recherche
"Géométrie Différentielle et Mécanique"

Onera Châtillon (France)
21 novembre 2025

[*] Conservatoire National des Arts et Métiers, LMSSC, Paris, France
[†] Laboratoire de Mathématiques d'Orsay, Université Paris-Saclay, France
[‡] Secihti/Tecnológico Nacional de México/I. T. Ensenada, Ensenada, Mexico

introduction aux intégrateurs variationnels

système dynamique non linéaire d'ordre deux :

$$m \, \frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \frac{\partial V}{\partial q}(q(t)) = 0$$

schéma du second ordre implicite de Nathan Newmark (1959) :

$$\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)_{j+1} = \left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)_j + \frac{h}{2}\left[\left(\frac{\mathrm{d}^2 q}{\mathrm{d}t^2}\right)_j + \left(\frac{\mathrm{d}^2 q}{\mathrm{d}t^2}\right)_{j+1}\right] + \mathrm{O}(h^2)$$

$$q_{j+1} = q_j + h\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)_j + \frac{h^2}{4}\left[\left(\frac{\mathrm{d}^2 q}{\mathrm{d}t^2}\right)_j + \left(\frac{\mathrm{d}^2 q}{\mathrm{d}t^2}\right)_{j+1}\right] + \mathrm{O}(h^3)$$

introduire l'impulsion $p \equiv m \, \frac{\mathrm{d}q}{\mathrm{d}t}$; alors $\frac{\mathrm{d}p}{\mathrm{d}t} + V'\big(q(t)\big) = 0$

$$p_{j+1} = p_j - \frac{h}{2}\left(V'_j + V'_{j+1}\right)$$

$$\begin{aligned} m\,(q_{j+1} - q_j) &= h\,p_j - \frac{h^2}{4}\left(V'_j + V'_{j+1}\right) \\ &= h\,p_j + \frac{h}{2}\,(p_{j+1} - p_j) = \frac{h}{2}\,(p_{j+1} + p_j) \end{aligned}$$

schéma de Newmark pour un oscillateur harmonique non linéaire :

$$\frac{p_{j+1} - p_j}{h} + \frac{1}{2}\left(V'_j + V'_{j+1}\right) = 0$$

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

le schéma de Newmark non linéaire est-il symplectique ?

réflexion initiée par Anthony Gravouil (novembre 2024)

schéma de Newmark

$$\frac{p_{j+1}-p_j}{h} + \frac{1}{2}\left(V'_{j+1} + V'_j\right) = 0, \qquad m\,\frac{q_{j+1}-q_j}{h} - \frac{1}{2}\left(p_{j+1} + p_j\right) = 0$$

système non linéaire à résoudre

$$p_{j+1} + \frac{h}{2}\,V'_{j+1} = p_j - \frac{h}{2}\,V'_j$$

$$m\,q_{j+1} - \frac{h}{2}\,p_{j+1} = m\,q_j + \frac{h}{2}\,p_j$$

différentier pour obtenir l'équation aux perturbations

$$\begin{pmatrix} 1 & \frac{h}{2}\,V''_{j+1} \\ -\frac{h}{2} & m \end{pmatrix} \begin{pmatrix} \delta p_{j+1} \\ \delta q_{j+1} \end{pmatrix} = \begin{pmatrix} 1 & -\frac{h}{2}\,V''_j \\ \frac{h}{2} & m \end{pmatrix} \begin{pmatrix} \delta p_j \\ \delta q_j \end{pmatrix}$$

les deux matrices ont-elles le même déterminant (cas scalaire !) ?

$$\det \begin{pmatrix} 1 & \frac{h}{2}\,V''_{j+1} \\ -\frac{h}{2} & m \end{pmatrix} = m + \frac{h^2}{4}\,V''_{j+1}$$

$$\det \begin{pmatrix} 1 & -\frac{h}{2}\,V''_j \\ \frac{h}{2} & m \end{pmatrix} = m + \frac{h^2}{4}\,V''_j$$

égalité dans le cas linéaire

intégrateur variationnel de point milieu

Lagrangian "continu" $\quad L = E_c - V$

énergie cinétique $\quad E_c = \frac{1}{2}\, m \left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2$

énergie potentialle $\quad V = V(q)$

$V(q) = \frac{1}{2}\, k\, q^2$ pour l'oscillateur harmonique (cas linéaire)

Lagrangien discret avec quadrature de point milieu

$$L_d \equiv L_d\,(q_\ell,\, q_r) = \int_{j\,h}^{(j+1)\,h} (E_c - V)\,\mathrm{d}t$$

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

action discrète

$$S_N = \sum_{j=0}^{j=N-1} L_d(q_j,\, q_{j+1})$$

integrateur variationnel

trouver des états discrets $q_j,\, q_{j+1}$ pour $0 \leq j \leq N-1$

de sorte que l'action discrète S_N est minimisée

intégrateur variationnel de point milieu *(ii)*

Lagrangien discret : $L_d = \frac{h}{2}\, m \left(\frac{q_r - q_\ell}{h}\right)^2 - h\, V\left(\frac{q_\ell + q_r}{2}\right)$

impulsion discrète

$$p_r = \frac{\partial}{\partial q_r} L_d(q_\ell, q_r) = m\, \frac{q_r - q_\ell}{h} - \frac{h}{2}\, V'\left(\frac{q_\ell + q_r}{2}\right)$$

$$p_{j+1} = \frac{\partial}{\partial q_r} L_d(q_j, q_{j+1}) = m\, \frac{q_{j+1} - q_j}{h} - \frac{h}{2}\, V'\left(\frac{q_j + q_{j+1}}{2}\right)$$

équations d'Euler-Lagrange

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

donc $\qquad p_j = -\frac{\partial}{\partial q_\ell} L_d(q_j, q_{j+1}) = m\, \frac{q_{j+1} - q_j}{h} + \frac{h}{2}\, V'\left(\frac{q_j + q_{j+1}}{2}\right)$

équations de Hamilton discrètes [Newmark]

$$\frac{p_{j+1} - p_j}{h} + V'\left(\frac{q_j + q_{j+1}}{2}\right) = 0 \qquad \frac{p_{j+1} - p_j}{h} + \frac{1}{2}\left(V'_j + V'_{j+1}\right) = 0$$

$$m\, \frac{q_{j+1} - q_j}{h} - \frac{1}{2}\left(p_j + p_{j+1}\right) = 0 \qquad m\, \frac{q_{j+1} - q_j}{h} - \frac{1}{2}\left(p_{j+1} + p_j\right) = 0$$

ce schéma est symplectique

$$\mathrm{d}p_{j+1} \wedge \mathrm{d}q_{j+1} = \mathrm{d}p_j \wedge \mathrm{d}q_j$$

intégrateur variationnel de degré un (Juan Simo)

Lagrangian "continu" $L = E_c - V$

énergie cinétique $E_c = \frac{1}{2}\, m \left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2$

énergie potentialle $V = V(q)$

interpolation interne de degré 1

$$q(\theta) = q_\ell\,(1-\theta) + q_r\,\theta, \quad \text{avec } t = j\,h + \theta\,h$$

calcul approché des intégrales avec la formule des trapèzes

$$\int_0^1 f(\theta)\,\mathrm{d}\theta \approx \frac{1}{2}\left(f(0) + f(1)\right)$$

Lagrangien discret

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

action discrète $S_N = \sum_{j=0}^{j=N-1} L_d\left(q_j,\, q_{j+1}\right)$

integrateur variationnel : minimiser l'action discrète S_N

intégrateur variationnel de degré un *(ii)*

Lagrangien discret

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

impulsion discrète

$$p_r = \frac{\partial}{\partial q_r} L_d(q_\ell, q_r) = m\, \frac{q_r - q_\ell}{h} - \frac{h}{2}\, V'(q_\ell)$$

$$p_{j+1} = \frac{\partial}{\partial q_r} L_d(q_j, q_{j+1}) = m\, \frac{q_{j+1} - q_j}{h} - \frac{h}{2}\, V'_{j+1}$$

équations d'Euler-Lagrange

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

donc $\qquad p_j = -\frac{\partial}{\partial q_\ell} L_d(q_j, q_{j+1}) = m\, \frac{q_{j+1} - q_j}{h} + \frac{h}{2}\, V'_j$

équations de Hamilton discrètes [point milieu]

$$\frac{p_{j+1} - p_j}{h} + \frac{1}{2}\left(V'_j + V'_{j+1}\right) = 0 \qquad\qquad \frac{p_{j+1} - p_j}{h} + V'\left(\frac{q_j + q_{j+1}}{2}\right) = 0$$

$$m\, \frac{q_{j+1} - q_j}{h} - \frac{p_j + p_{j+1}}{2} - \frac{h}{4}\left(V'_{j+1} - V'_j\right) = 0 \qquad m\, \frac{q_{j+1} - q_j}{h} - \frac{p_j + p_{j+1}}{2} = 0$$

l'intégrateur variationnel de degré un est symplectique

équations de Hamilton discrètes

$$\frac{p_{j+1}-p_j}{h} + \frac{1}{2}\left(V'_j + V'_{j+1}\right) = 0$$

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

système non linéaire à résoudre

$$p_{j+1} + \frac{h}{2}\,V'_{j+1} = p_j - \frac{h}{2}\,V'_j$$

$$m\,q_{j+1} - \frac{h}{2}\,p_{j+1} - \frac{h^2}{4}\,V'_{j+1} = m\,q_j + \frac{h}{2}\,p_j - \frac{h^2}{4}\,V'_j$$

différentier pour obtenir l'équation aux perturbations

$$\begin{pmatrix} 1 & \frac{h}{2}V''_{j+1} \\ -\frac{h}{2} & m - \frac{1}{4}\,h^2\,V''_{j+1} \end{pmatrix}\begin{pmatrix} \delta p_{j+1} \\ \delta q_{j+1} \end{pmatrix} = \begin{pmatrix} 1 & -\frac{h}{2}V''_j \\ \frac{h}{2} & m - \frac{1}{4}\,h^2\,V''_j \end{pmatrix}\begin{pmatrix} \delta p_j \\ \delta q_j \end{pmatrix}$$

les deux matrices ont-elles le même déterminant ?

oui ! (il vaut m)

le schéma est symplectique : $\mathrm{d}p_{j+1} \wedge \mathrm{d}q_{j+1} = \mathrm{d}p_j \wedge \mathrm{d}q_j$

numérique du principe de moindre action

René De Vogelaere, "Methods of integration which preserve the contact transformation property of the Hamilton equations", non publié, 1956

METHODS OF INTEGRATION WHICH PRESERVE
THE CONTACT TRANSFORMATION PROPERTY
OF THE HAMILTON EQUATIONS
(Internal Classification: me 2.4, pr 5.2, pr 5.4)

RENE DEVOGELAERE
DEPARTMENT OF MATHEMATICS
APRIL, 1956

curate.nd.edu

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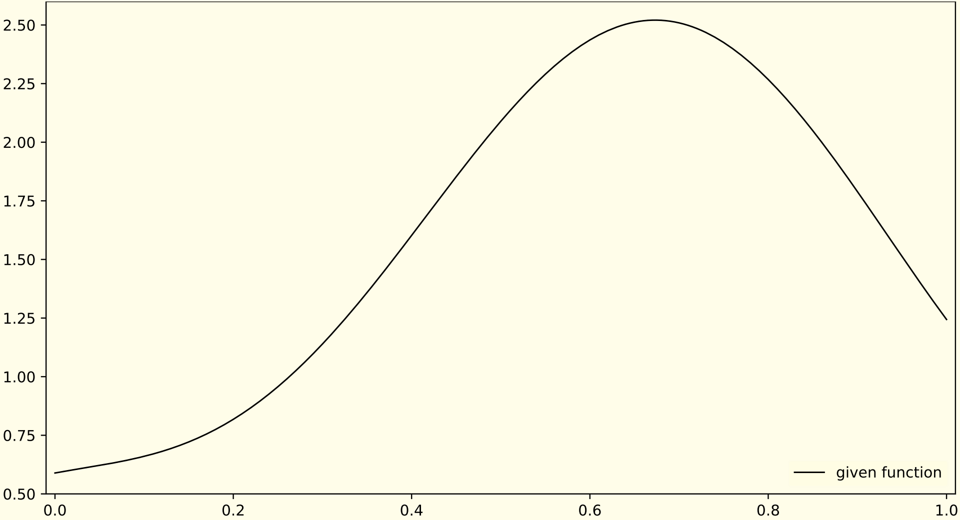
J. M. Wendlandt, J. E. Marsden, "Mechanical integrators derived from a discrete variational principle", *Physica D*, 1997

J. E. Marsden, M. West, "Discrete mechanics and variational integrators", *Acta Numerica*, 2001

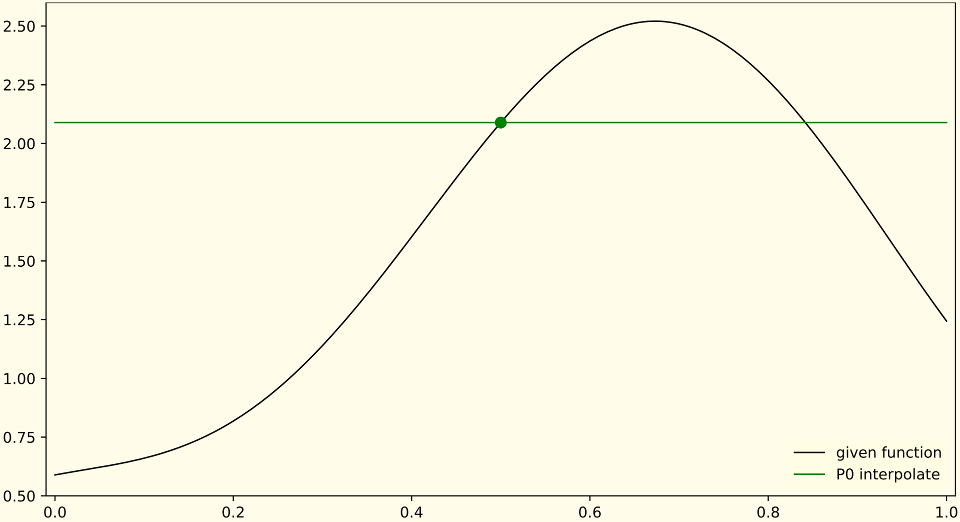
E. Hairer, C. Lubich, G. Wanner, *Geometric numerical integration, structure-preserving algorithms for ordinary differential equations*, 2006

outline

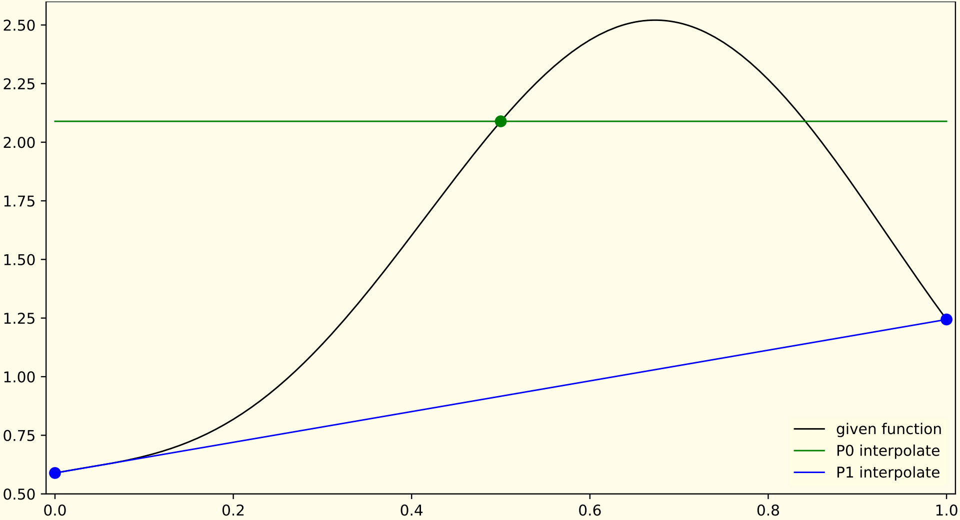
polynomial interpolation: initial function



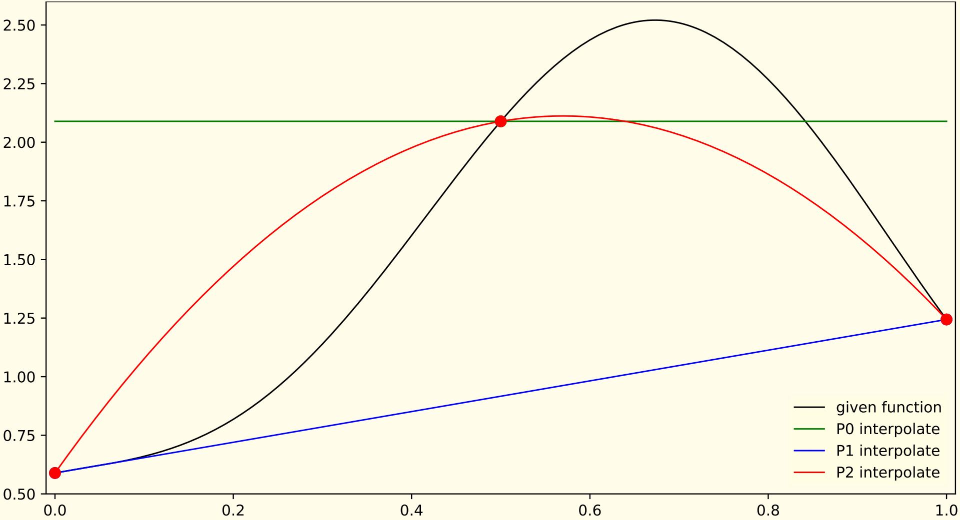
polynomial interpolation: degree zero



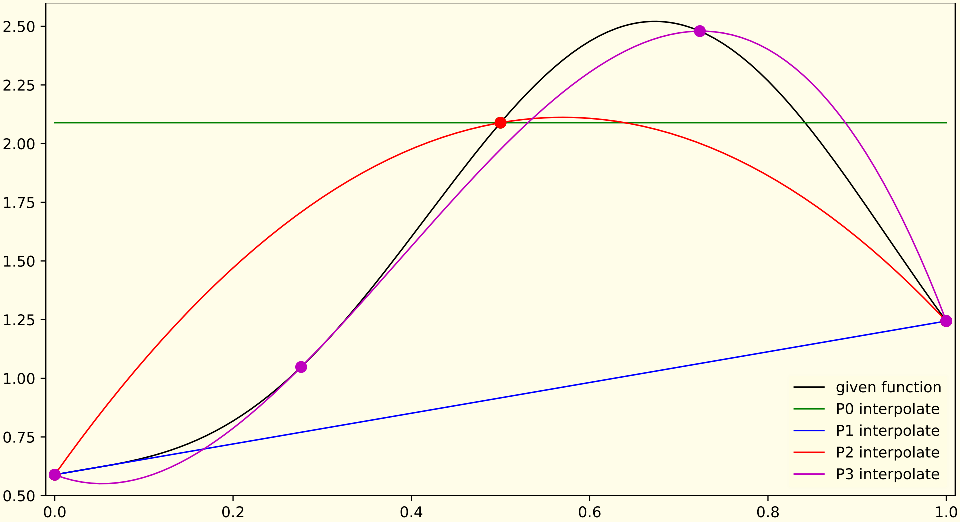
polynomial interpolation: degree one



polynomial interpolation: degree two



polynomial interpolation: degree three

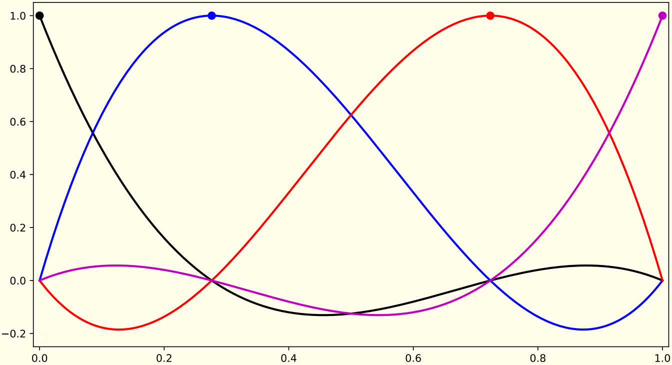


basis functions for degree 3 interpolation

$$f_3(\theta) = f_\ell\ \varphi_0(\theta) + f_\xi\ \varphi_\xi(\theta) + f_{1-\xi}\ \varphi_{1-\xi}(\theta) + f_r\ \varphi_1(\theta)$$

$$\begin{aligned}
\varphi_0(\theta) &= 5(\theta-\xi)\,(\theta-(1-\xi))\,(1-\theta) \\
\varphi_\xi(\theta) &= -5\sqrt{5}\ \theta\,(1-\theta)\,(\theta-(1-\xi)) \\
\varphi_{1-\xi}(\theta) &= 5\sqrt{5}\,\theta\,(1-\theta)\,(\theta-\xi) \\
\varphi_1(\theta) &= 5\,\theta\,(\theta-\xi)\,(\theta-(1-\xi))
\end{aligned}$$

$$\xi = \frac{1}{2} - \frac{\sqrt{5}}{10}$$



Lobatto's numerical integration of degree 3

interpolate a function from the 4 values $f_\ell, \; f_\xi, \; f_{1-\xi}, \; f_r$

polynomial of degree 3

$$f \approx f_3(\theta) = f_\ell \; \varphi_0(\theta) + f_\xi \; \varphi_\xi(\theta) + f_{1-\xi} \; \varphi_{1-\xi}(\theta) + f_r \; \varphi_1(\theta)$$

evaluate the integral of the function on the interval $[0, 1]$

$$\int_0^1 f(\theta) \, \mathrm{d}\theta \approx \int_0^1 f_3(\theta) \, \mathrm{d}\theta$$

the computation of the integral is exact for the function f_3

$$\int_0^1 f_3(\theta) \, \mathrm{d}\theta = f_\ell \; \int_0^1 \varphi_0(\theta) \, \mathrm{d}\theta + f_\xi \; \int_0^1 \varphi_\xi(\theta) \, \mathrm{d}\theta + f_{1-\xi} \; \int_0^1 \varphi_{1-\xi}(\theta) \, \mathrm{d}\theta + f_r \; \int_0^1 \varphi_1(\theta) \, \mathrm{d}\theta$$

Lobatto's quadrature formula

$$\int_0^1 f(\theta) \, \mathrm{d}\theta \approx \frac{1}{12} \left(f_\ell + f_r \right) + \frac{5}{12} \left(f_\xi + f_{1-\xi} \right)$$

this relation is **exact** if f is a polynomial function of degree ≤ 5

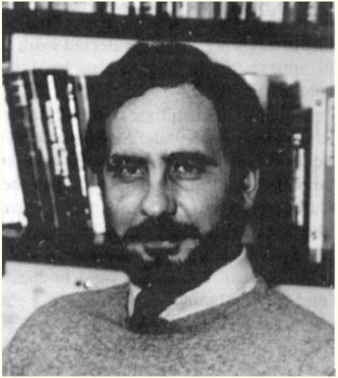
numerical integration for variational schemes

degree of internal interpolation

1

2

3



Juan Simo
(1952-1994)

Thomas Simpson
(1710-1761)

Rehuel Labatto
(1797-1866)

3rd degree dynamic data interpolation

time step $h = \frac{T}{N}$

inside the interval $[j\,h,\,(j+1)\,h]$, $t = j\,h + \theta\,h$ with $0 \leq \theta \leq 1$

interpolate an unknown state function:

$$q(t) \approx q_\ell\ \varphi_0(\theta) + q_\xi\ \varphi_\xi(\theta) + q_{1-\xi}\ \varphi_{1-\xi}(\theta) + q_r\ \varphi_1(\theta)$$

differentiate relative to time:

$$\frac{\mathrm{d}q}{\mathrm{d}t}(t) \approx \frac{1}{h}\left[q_\ell\,\varphi_0'(\theta) + q_\xi\,\varphi_\xi'(\theta) + q_{1-\xi}\,\varphi_{1-\xi}'(\theta) + q_r\,\varphi_r'(\theta)\right]$$

discrete gradients at nodal points

$$\frac{\mathrm{d}q}{\mathrm{d}t}(j\,h) \approx g_\ell,\ \frac{\mathrm{d}q}{\mathrm{d}t}((j+\xi)\,h) \approx g_\xi,\ \frac{\mathrm{d}q}{\mathrm{d}t}((j+1-\xi)\,h) \approx g_{1-\xi},$$
$$\frac{\mathrm{d}q}{\mathrm{d}t}((j+1)\,h) \approx g_r$$

$$g_\ell = \frac{1}{h}\left[q_\ell\,\varphi_0'(0) + q_\xi\,\varphi_\xi'(0) + q_{1-\xi}\,\varphi_{1-\xi}'(0) + q_r\,\varphi_r'(0)\right]$$
$$g_\xi = \frac{1}{h}\left[q_\ell\,\varphi_0'(\xi) + q_\xi\,\varphi_\xi'(\xi) + q_{1-\xi}\,\varphi_{1-\xi}'(\xi) + q_r\,\varphi_r'(\xi)\right]$$
$$g_{1-\xi} = \frac{1}{h}\left[q_\ell\,\varphi_0'(1-\xi) + q_\xi\,\varphi_\xi'(1-\xi) + q_{1-\xi}\,\varphi_{1-\xi}'(1-\xi) + q_r\,\varphi_r'(1-\xi)\right]$$
$$g_r = \frac{1}{h}\left[q_\ell\,\varphi_0'(1) + q_\xi\,\varphi_\xi'(1) + q_{1-\xi}\,\varphi_{1-\xi}'(1) + q_r\,\varphi_r'(1)\right]$$

discrete Lagrangian

continuous Lagrangian $\quad L = E_c - V$

kinetic energy $\quad E_c = \frac{1}{2}\, m \left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2$

potential energy $\quad V = V(q)$

$V(q) = \frac{1}{2}\, k\, q^2$ in the linear case of an harmonic oscillator

discrete Lagrangian

$$L_d \equiv L_d\,(q_\ell,\, q_\xi,\, q_{1-\xi},\, q_r) = \int_{j\,h}^{(j+1)\,h} (E_c - V)\ \mathrm{d}t$$

$$L_d = \frac{h}{2}\, m \left[\frac{1}{12}\left(g_\ell^2 + g_r^2\right) + \frac{5}{12}\left(g_\xi^2 + g_{1-\xi}^2\right)\right]$$
$$-h \left[\frac{1}{12}\left(V(q_\ell) + V(q_r)\right) + \frac{5}{12}\left(V(q_\xi) + V(q_{1-\xi})\right)\right]$$

discrete action

$$S_N = \sum_{j=0}^{j=N-1} L_d\left(q_j,\, q_{j+\xi},\, q_{j+1-\xi},\, q_{j+1}\right)$$

variational integrator

find a discrete state set by $q_j,\, q_{j+\xi},\, q_{j+1-\xi},\, q_{j+1}$ for $0 \le j \le N-1$

such that the discrete action S_N is minimized

local elimination of degrees of freedom

discrete action $\quad S_N = \sum_{j=0}^{j=N-1} L_d\big(q_j,\, q_{j+\xi},\, q_{j+1-\xi},\, q_{j+1}\big)$

discrete state set by $q_j,\, q_{j+\xi},\, q_{j+1-\xi},\, q_{j+1}$ for $0 \le j \le N-1$

such that the discrete action S_N is minimized

the internal degrees of freedon $q_{j+\xi}$ and $q_{j+1-\xi}$

are internal to the interval $[j\,h,\, (j+1)\,h]$

reduced Lagrangian

$$L_r(q_\ell,\, q_r) = \min_{q_\xi,\, q_{1-\xi}} L_d\big(q_\ell,\, q_\xi,\, q_{1-\xi},\, q_r\big)$$

explicit expressions for the harmonic oscillator with $V(q) = \frac{1}{2}\, m\,\omega^2\, q^2$

determinant $\delta = (h^2\omega^2 - 30)\,(h^2\omega^2 - 10)$

$\delta > 0 \quad \text{for} \quad 0 < h\,\omega < \sqrt{10}$: natural stability condition

$$q_\xi = \frac{1}{\delta}\big[-5\,\big(h^2\omega^2 - 30\big)\,(q_r + q_\ell) + 3\sqrt{5}\big(h^2\omega^2 - 10\big)(q_r - q_\ell)\big]$$

$$q_{1-\xi} = \frac{1}{\delta}\big[-5\,\big(h^2\omega^2 - 30\big)\,(q_r + q_\ell) - 3\sqrt{5}\,\big(h^2\omega^2 - 10\big)\,(q_r - q_\ell)\big]$$

harmonic oscillator: sixth order accuracy

Euler-Lagrange equations

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

harmonic oscillator: $V(q) = \frac{1}{2}\, m\, \omega^2\, q^2$

$$(*) \quad \left\{ \begin{array}{l} \frac{1}{h^2}\,(q_{j-1} - 2q_j + q_{j+1}) + \frac{\omega^2}{30}(q_{j-1} + 28q_j + q_{j+1}) \\ \qquad + \frac{\omega^4\, h^2}{1800}\,(q_{j-1} - 92q_j + q_{j+1}) + \frac{\omega^6\, h^4}{1800}\, q_j = 0 \end{array} \right.$$

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \omega^2\, q = \mathrm{O}(h^2) \ ?$$

truncation error

replace the discrete variables q_{j+1}, q_j and q_{j-1}

by the solution of the differential equation $\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \omega^2\, q = 0$

$$q_{j+1} = q_j + h\,\frac{\mathrm{d}q}{\mathrm{d}t} + \frac{h^2}{2}\,\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} + \frac{h^3}{6}\,\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} + \frac{h^4}{24}\,\frac{\mathrm{d}^4 q}{\mathrm{d}t^4} + \frac{h^5}{120}\,\frac{\mathrm{d}^5 q}{\mathrm{d}t^5} + \frac{h^6}{720}\,\frac{\mathrm{d}^6 q}{\mathrm{d}t^6} + \mathrm{O}(h^7)$$

$$q_{j-1} = q_j - h\,\frac{\mathrm{d}q}{\mathrm{d}t} + \frac{h^2}{2}\,\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} - \frac{h^3}{6}\,\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} + \frac{h^4}{24}\,\frac{\mathrm{d}^4 q}{\mathrm{d}t^4} - \frac{h^5}{120}\,\frac{\mathrm{d}^5 q}{\mathrm{d}t^5} + \frac{h^6}{720}\,\frac{\mathrm{d}^6 q}{\mathrm{d}t^6} + \mathrm{O}(h^7)$$

the left-hand side of equation $(*)$ does not vanish

but defines the truncation error $\mathcal{T}_h(q_j)$

we have $\mathcal{T}_h(q_j) = -\frac{1}{21600}\,\omega^8\, h^6\, q_j + \mathrm{O}(h^8)$.

harmonic oscillator: stability condition

Euler-Lagrange equations

$$(*) \quad \left\{ \begin{array}{l} \frac{1}{h^2}\,(q_{j-1} - 2q_j + q_{j+1}) + \frac{\omega^2}{30}(q_{j-1} + 28q_j + q_{j+1}) \\ \qquad + \frac{\omega^4\,h^2}{1800}\,(q_{j-1} - 92q_j + q_{j+1}) + \frac{\omega^6\,h^4}{1800}\,q_j = 0 \end{array} \right.$$

characteristic polynomial for equation $(*)$

$$\frac{1}{h^2}\left(1 - 2r + r^2\right) + \frac{\omega^2}{30}\left(1 + 28r + r^2\right) + \frac{\omega^4 h^2}{1800}\left(1 - 92r + r^2\right) + \frac{\omega^6 h^4}{1800} r = 0$$

corresponding discriminant

$$\Delta = \frac{\omega^2}{h^2}\left(h^2\omega^2 - 10\right)\left(h^2\omega^2 - 30\right)\left(h^2\omega^2 - 60\right)\left(h^4\omega^4 - 84\,h^2\omega^2 + 720\right)$$

polynomial $\left(h^4\omega^4 - 84\,h^2\omega^2 + 720\right)$ has two real roots

$$\Delta < 0 \quad \text{when} \quad 0 < h\,\omega < \sqrt{6\,(7 - \sqrt{29})} \approx \sqrt{9.689} \approx 3.11$$

stability condition $0 < h\,\omega < 3.11$

a little more than two points per period of oscillation

harmonic oscillator: symplectic structure

quadratic potential $\quad V(q) = \frac{1}{2}\, m\, \omega^2\, q^2$

right-hand generalized moment $\quad p_r = \frac{\partial L_r}{\partial q_r}(q_\ell, q_r) = p_{j+1}$

determinant $\quad \delta = (h^2\omega^2 - 30)\,(h^2\omega^2 - 10)$

$$p_r = m\frac{q_r - q_\ell}{h} + \frac{m}{6\,\delta}\left[-300\, h\, \omega^2\, (q_\ell + 2\, q_r) + 5\, h^3\, \omega^4\, (q_\ell + 8\, q_r) - \frac{1}{2}\, h^5\, \omega^6 q_r\right]$$

Euler-Lagrange equation $\quad p_j = -\frac{\partial L_r}{\partial q_\ell}(q_j,\, q_{j+1})$

discrete Hamilton equations

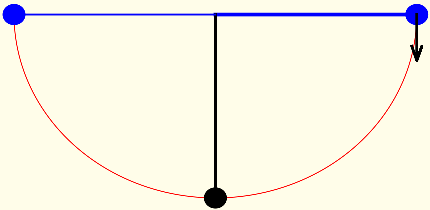
$$\frac{p_{j+1} - p_j}{h} + m\, \omega^2\, \frac{(60 - h^2\, \omega^2)}{6\, (10 - h^2\, \omega^2)}\left(\frac{q_j + q_{j+1}}{2}\right) = 0$$

$$m\, \frac{q_{j+1} - q_j}{h} - 24\, \frac{30 - h^2\, \omega^2}{h^4\, \omega^4 - 84 h^2\, \omega^2 + 720}\left(\frac{p_j + p_{j+1}}{2}\right) = 0$$

symplectic scheme $\quad \begin{pmatrix} p_{j+1} \\ q_{j+1} \end{pmatrix} = \mathbf{\Phi} \begin{pmatrix} p_j \\ q_j \end{pmatrix} \quad$ with $\det \mathbf{\Phi} = 1$

preservation of a discrete energy $\quad H_d \approx \frac{1}{2\, m}\, p^2 + m\, \frac{\omega^2}{2}\, q^2$

first numerical experiments



harmonic oscillator or nonlinear pendulum

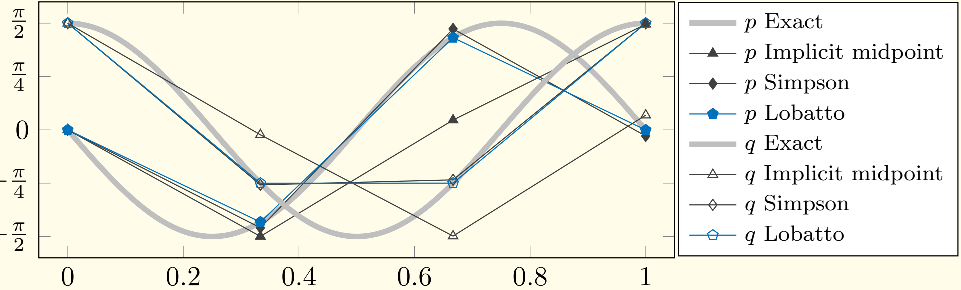
initial conditions: $q(0) = \frac{\pi}{2}$; $p(0) = 0$

analytical references:

trigonometric functions

Jacobi elliptic functions (see *e.g.* A. Chenciner (2000))

harmonic oscillator: numerical experiments



one period, $N = 3$ mesh points

[momentum data have been rescaled]

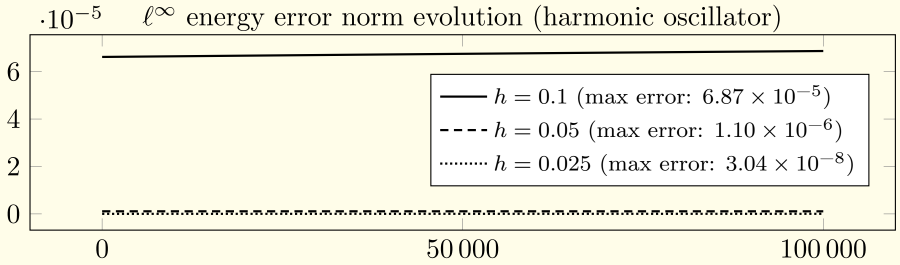
harmonic oscillator: mesh convergence

errors for the discrete maximum norm

number of meshes	10	20	40	order
momentum p	$8.952\ 10^{-6}$	$1.393\ 10^{-7}$	$2.170\ 10^{-9}$	6
state q	$7.640\ 10^{-7}$	$1.194\ 10^{-8}$	$1.876\ 10^{-10}$	6
energy $H(p, q)$	$6.619\ 10^{-5}$	$1.098\ 10^{-6}$	$1.699\ 10^{-8}$	6
discrete energy $H_d(p, q)$	$2.665\ 10^{-15}$	$1.332\ 10^{-15}$	$2.220\ 10^{-15}$	exact

integration time: 5 periods

harmonic oscillator: long time integration



integration time: 10^5 periods

the error for the total energy remains **bounded**

it tends to zero at 6th order for the Lobatto scheme ?

very basic ideas!

work unknown to our team until April 2025

Sina Ober-Blöbaum and Nils Saake
"Construction and analysis of higher order
Galerkin variational integrators"
Advances in Computational Mathematics, 2015

very similar ideas presented in a completely different way

numerical convergence for a harmonic oscillator
with symplectic schemes of accuracy up to order 10

choosing a nonlinear pendulum
so as not to merely reproduce already known results

nonlinear pendulum: numerical scheme

discrete Lagrangian

$$L_d = \frac{h}{2}\, m \left[\frac{1}{12}\left(g_\ell^2 + g_r^2\right) + \frac{5}{12}\left(g_\xi^2 + g_{1-\xi}^2\right)\right] - \frac{h}{12}\left[V_\ell + V_r + 5\left(V_\xi + V_{1-\xi}\right)\right]$$

with $V_\ell = V(q_\ell),\ V_\xi = V(q_\xi),\ V_{1-\xi} = V(q_{1-\xi}),\ V_r = V(q_r)$

$$L_d = \frac{m}{12\,h}\Big[26\ \left({q_\ell}^2 + {q_r}^2\right) - 2\, q_\ell q_r + 50\left({q_\xi}^2 - q_\xi q_{1-\xi} + {q_{1-\xi}}^2\right)$$
$$-25\,(q_\ell + q_r)(q_\xi + q_{1-\xi}) - 15\sqrt{5}(q_\ell - q_r)(q_\xi - q_{1-\xi})\Big]$$
$$-\frac{h}{12}\left[V_\ell + 5\left(V_\xi + V_{1-\xi}\right) + V_r\right]$$

discrete equations for the internal variables: $\frac{\partial L_d}{\partial q_\xi} = 0,\ \frac{\partial L_d}{\partial q_{1-\xi}} = 0$

$$q_\xi - \frac{h^2}{30\,m}\left(V'_{1-\xi} + 2V'_\xi\right) = \frac{5+\sqrt{5}}{10} q_\ell + \frac{5-\sqrt{5}}{10} q_r$$
$$q_{1-\xi} - \frac{h^2}{30\,m}\left(2V'_{1-\xi} + V'_\xi\right) = \frac{5-\sqrt{5}}{10} q_\ell + \frac{5+\sqrt{5}}{10} q_r$$

with $V'_x \equiv \left(\frac{\partial V}{\partial q}\right)(q_x)$

the evaluation of $L_r(q_\ell,\, q_r)$ needs the implicit function theorem

nonlinear pendulum: numerical scheme *(ii)*

Euler-Lagrange equations

$$\frac{\partial L_d}{\partial q_r}\big(q_{j-1},\, q_{j-1+\xi},\, q_{j-\xi},\, q_j\big) + \frac{\partial L_d}{\partial q_\ell}\big(q_j,\, q_{j+\xi},\, q_{j+1-\xi},\, q_{j+1}\big) = 0$$

or equivalently $\quad \frac{\partial L_r}{\partial q_r}\big(q_{j-1},\, q_j\big) + \frac{\partial L_r}{\partial q_\ell}\big(q_j,\, q_{j+1}\big) = 0$

$$\frac{1}{h^2}\left(q_{j-1} - 2q_j + q_{j+1}\right) + \frac{1}{24m}\Big[(5-\sqrt{5})\, V'_{j-1+\xi} + (5+\sqrt{5})\, V'_{j-\xi} + 4V'_j + (5+\sqrt{5})\, V'_{j+\xi} + (5-\sqrt{5}) V'_{j+1-\xi}\Big] = 0$$

right-hand generalized moment

$$p_r = \frac{\partial L_r}{\partial q_r}\big(q_\ell, q_r\big) = \frac{\partial L_d}{\partial q_r}\big(q_\ell, q_\xi,\, q_{1-\xi},\, q_r\big) = p_{j+1}$$

then $\quad p_j = -\frac{\partial L_d}{\partial q_\ell}\big(q_j,\, q_{j+\xi},\, q_{j+1-\xi},\, q_{j+1}\big)$

discrete Hamiltonian dynamics

$$\frac{1}{h}\big(p_{j+1} - p_j\big) + \frac{1}{12}\Big[V'_j + 5\left(V'_{j+\xi} + V'_{j+1-\xi}\right) + V'_{j+1}\Big] = 0$$

$$m\left(q_{j+1} - q_j\right) - \frac{h}{2}\big(p_j + p_{j+1}\big) = \frac{h^2}{24}\Big[V'_{j+1} + \sqrt{5}\left(V'_{j+1-\xi} - V'_{j+\xi}\right) - V'_j\Big]$$

nonlinear pendulum: numerical scheme *(iii)*

internal degrees of freedom

$$q_{j+\xi} - \frac{h^2}{30\,m}\left(V'_{j+1-\xi} + 2V'_{j+\xi}\right) = \frac{5+\sqrt{5}}{10}\,q_j + \frac{5-\sqrt{5}}{10}\,q_{j+1}$$

$$q_{j+1-\xi} - \frac{h^2}{30\,m}\left(2V'_{j+1-\xi} + V'_{j+\xi}\right) = \frac{5-\sqrt{5}}{10}\,q_j + \frac{5+\sqrt{5}}{10}\,q_{j+1}$$

discrete Hamiltonian dynamics

$$p_{j+1} - p_j + \frac{h}{12}\left[V'_j + 5\left(V'_{j+\xi} + V'_{j+1-\xi}\right) + V'_{j+1}\right] = 0$$

$$q_{j+1} - q_j - \frac{h^2}{24m}\left[V'_{j+1} + \sqrt{5}\left(V'_{j+1-\xi} - V'_{j+\xi}\right) - V'_j\right] - \frac{h}{2m}(p_{j+1} + p_j) = 0$$

nonlinear system of 4 equations with 4 unknowns

$$F_L\left(q_{j+\xi},\, q_{j+1-\xi},\, p_{j+1},\, q_{j+1}\right) = 0$$

Newton iterations with

$$\mathrm{d}F_L = \begin{pmatrix} 1 - \frac{h^2}{15m}V''_\xi & -\frac{h^2}{30m}V''_{1-\xi} & 0 & \frac{-5+\sqrt{5}}{10} \\ -\frac{h^2}{30m}V''_{1-\xi} & 1 - \frac{h^2}{15m}V''_{1-\xi} & 0 & -\frac{5+\sqrt{5}}{10} \\ \frac{5h}{12}V''_\xi & \frac{5h}{12}V''_{1-\xi} & 1 & \frac{h}{12}V''(q) \\ \frac{\sqrt{5}h^2}{24m}V''_\xi & -\frac{\sqrt{5}h^2}{24m}V''_{1-\xi} & -\frac{h}{2m} & 1 - \frac{h^2}{24m}V''(q) \end{pmatrix}$$

nonlinear pendulum: symplectic structure

differentiate the equations for the internal degrees of freedom

$$\delta q_{j+\xi} = \frac{1}{\Delta}\Big[30\,m^2\,\big((5+\sqrt{5})\,\delta q_j - (-5+\sqrt{5})\,\delta q_{j+1}\big)$$
$$-m\,h^2\,V''_{j+1-\xi}\big((5+3\sqrt{5})\,\delta q_j + (5-3\sqrt{5})\,\delta q_{j+1}\big)\Big]$$
$$\delta q_{j+1-\xi} = \frac{1}{\Delta}\Big[-30\,m^2\,\big((-5+\sqrt{5})\,\delta q_j - (5+\sqrt{5})\,\delta q_{j+1}\big)$$
$$-m\,h^2\,V''_{j+\xi}\big((5-3\sqrt{5})\,\delta q_j + (5+3\sqrt{5})\,\delta q_{j+1}\big)\Big]$$
$$\Delta = 300\,m^2 - 20\,m\,h^2\,(V''_{j+\xi} + V''_{j+1-\xi}) + h^4\,V''_{j+\xi}\,V''_{j+1-\xi}$$

differentiate the discrete Hamilton equations

replace $\delta q_{j+\xi}$ and $\delta q_{j+1-\xi}$ by their values

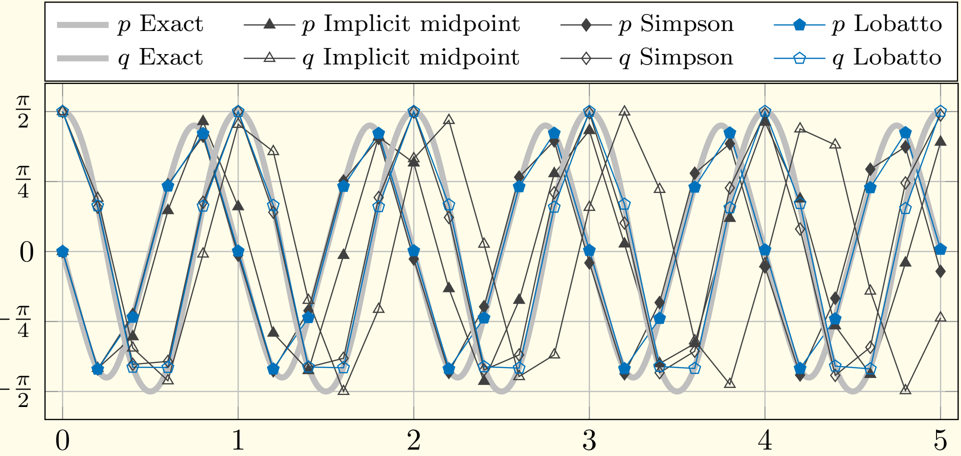
then $\quad A\begin{pmatrix}\delta p\\ \delta q\end{pmatrix}_{j+1} = B\begin{pmatrix}\delta p\\ \delta q\end{pmatrix}_j$

$$\det A = \det B = \frac{1}{6\Delta}\Big[1800\,m^2 + 30\,m\,h^2\,(V''_{j+\xi} + V''_{j+1-\xi}) + h^4\,V''_{j+\xi}\,V''_{j+1-\xi}\Big]$$

the relation $\quad \frac{\partial p_{j+1}}{\partial p_j}\frac{\partial q_{j+1}}{\partial q_j} - \frac{\partial p_{j+1}}{\partial q_j}\frac{\partial q_{j+1}}{\partial p_j} = 1 \quad$ is established

the Lobatto scheme defined page 25 is symplectic

nonlinear pendulum: momentum and state evolutions



5 periods, $N = 5$ mesh points per period

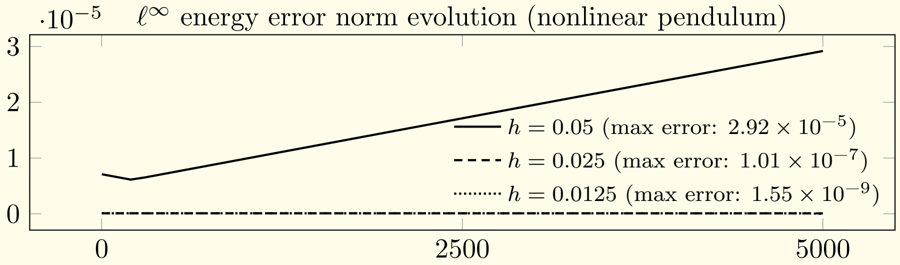
nonlinear pendulum: mesh convergence

errors for the discrete maximum norm

number of meshes	50	100	200	order
momentum p	$2.832\ 10^{-9}$	$4.567\ 10^{-11}$	$7.070\ 10^{-13}$	6
state q	$4.218\ 10^{-10}$	$6.692\ 10^{-12}$	$1.057\ 10^{-13}$	6
energy $H(p, q)$	$6.234\ 10^{-10}$	$1.028\ 10^{-11}$	$1.589\ 10^{-13}$	6

integration time: 5 periods

nonlinear pendulum: long time integration



integration time: 10^5 periods

ℓ^∞ energy error growth rate

$4.77\,10^{-9}$ when $h = 0.05$
$2.36\,10^{-12}$ when $h = 0.025$
$1.02\,10^{-17}$ when $h = 0.0125$.

conclusion

sixth-order variational integrator

Lobatto's quadrature (cubic Lagrange polynomials)

least action principle

harmonic oscillator

nonlinear integrator tested on the nonlinear pendulum

symplectic and conditionally stable method

future work: top, multi-degrees of freedom

references with Juan-Antonio Rojas-Quintero

"A variational symplectic scheme based on Lobatto's quadrature"
7th international conference on Geometric Science of Information, Saint-Malo, 29 - 31 october 2025
Lecture Notes in Computer Science, volume 16034, pages 332-342.

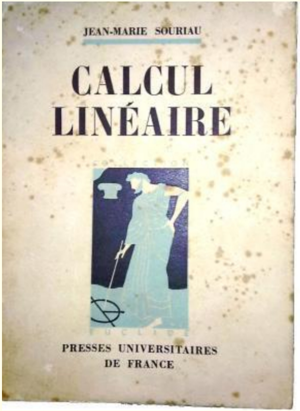
"Simpson's variational integrator for systems with quadratic Lagrangians", with José Guadalupe Cabrera-Díaz
Axioms, volume 12, article 255, 2024.

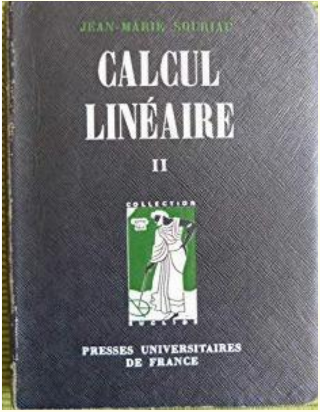
"Simpson's quadrature for a nonlinear variational symplectic scheme"
Finite Volumes for Complex Applications X
Strasbourg, 30 october - 03 november 2023.
Springer Proceedings in Mathematics & Statistics, volume 433, pages 83-92, 2023.

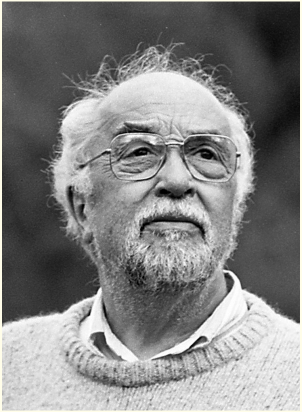
"A variational symplectic scheme based on Simpson's quadrature"
6th international conference on Geometric Science of Information, Saint-Malo, 30 august - 01 september 2023.
Lecture Notes in Computer Science, volume 14072, pages 22-31, 2023.

Juan Rojas au Souriau Colloquium, Bastia, mai 2024

Jean-Marie-Souriau et la géométrie symplectique







cours à l'École Spéciale des Travaux Aéronautiques

    “École des Meuniers”

        “Méthodes nouvelles de la Physique mathématique” (≈ 1948)

ingénieur à l'ONERA

    “Sur la stabilité des avions”, Thèse d'État (1952)

merci de votre attention !

onera.fr

bonus : symplecticité discrète

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: $a^{\mathrm{t}} d - c^{\mathrm{t}} b = \mathrm{I}$.

Proposition 2 [Lewis & Simo (1995), Wendlandt & Marsden (1997)]

A numerical scheme obtained with a discrete set of Euler-Lagrange equations is symplectic.

discrete symplecticity *(ii)*

Proof of Proposition 1

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

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

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

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

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

(i) $a^{\mathrm{t}}c$ 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: $a^{\mathrm{t}}d - c^{\mathrm{t}}b = \mathrm{I}$

then

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

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

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

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 $a = \gamma^{-1}$. $\square$

jmsouriau.com