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A variational symplectic scheme based on Simpson's quadrature

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Abstract

We propose a variational symplectic numerical method for the time integration of dynamical systems issued from the least action principle. We assume a quadratic internal interpolation of the state and we approximate the action in a small time step by the Simpson's quadrature formula. The resulting scheme is explicit for an elementary harmonic oscillator. It is a stable, explicit, and symplectic scheme satisfying the conservation of an approximate energy. Numerical tests illustrate our theoretical study.

1) Introduction

The principle of least action is a key point for establishing evolution equations or partial differential equations, from classical to quantum mechanics and electromagnetisms [1, 3, 12]. An important application of this principle is proposed with the finite element method [2] and it is used for engineering applications since the 1950's. For dynamics equations and dynamical systems, a synthesis of the state of the art is proposed in [5, 11, 13].

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In this contribution, we first recall the classical variational approach. It is founded on a midpoint quadrature formula for the approximate calculation of an integral. We essentially follow the contribution [6] in this Section 2. Then we recall in Section 3 the interpolation of functions with quadratic finite elements. Once this prerequisite is in place, we develop in Section 4 the approximation of discrete Lagrangians with Simpson's quadrature formula. The result is a numerical scheme that can be considered as a variant of the classical approach presented in Section 2 and we derive in Section 5 the discrete Euler-Lagrange equations. We notice in Section 6 that the scheme admits a symplectic structure and in Section 7 that an approximation of the energy is conserved along the discrete time integration. First numerical results are presented in Section 8 before some words of conclusion.

2) A classical variational symplectic numerical scheme

We consider a dynamical system described by a state $q(t)$ composed by a simple real variable to fix the ideas, and for $0 \leq t \leq T$. The continuous action S_c introduces a Lagrangian L and we have

$$(1) \quad S_c = \int_0^T L\left(\frac{dq}{dt}, q(t)\right) dt.$$

We use in this contribution a very classical Lagrangian

$$(2) \quad L\left(\frac{dq}{dt}, q\right) = \frac{m}{2} \left(\frac{dq}{dt}\right)^2 - V(q).$$

A discretization of the relation (1) is obtained by splitting the interval $[0, T]$ into N elements and we set $h = \frac{T}{N}$. At the discrete time $t_j = jh$, an approximation q_j of $q(t_j)$ is introduced and a discrete form S_d of the continuous action S_c can be defined according to

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

The discrete Lagrangian $L_d(q_\ell, q_r)$ is derived from the relation (2) with a centered finite difference approximation $\frac{dq}{dt} \simeq \frac{q_r - q_\ell}{h}$ and a midpoint quadrature formula

$$(3) \quad \int_0^h V(q(t)) dt \simeq h V\left(\frac{q_\ell + q_r}{2}\right) : \\ L_d(q_\ell, q_r) = \frac{mh}{2} \left(\frac{q_r - q_\ell}{h}\right)^2 - h V\left(\frac{q_\ell + q_r}{2}\right).$$

We observe that $S_d = \dots + L_d(q_{j-1}, q_j) + L_d(q_j, q_{j+1}) + \dots$. Then the discrete Euler Lagrange equation $\delta S_d = 0$ for an arbitrary variation δq_j of the discrete variable q_j can be written

$$(4) \quad \frac{\partial L_d}{\partial q_r}(q_{j-1}, q_j) + \frac{\partial L_d}{\partial q_\ell}(q_j, q_{j+1}) = 0.$$

Taking into account the relation (3), we obtain

$$(5) \quad m \frac{q_{j+1} - 2q_j + q_{j-1}}{h^2} + \frac{1}{2} \left[\frac{dV}{dq}\left(\frac{q_j + q_{j+1}}{2}\right) + \frac{dV}{dq}\left(\frac{q_{j-1} + q_j}{2}\right) \right] = 0.$$

This numerical scheme is clearly consistent with the second order differential equation

$$(6) \quad m \frac{d^2q}{dt^2} + \frac{dV}{dq} = 0$$

associated with the Lagrangian proposed in (2). It is easy to verify that when

$$(7) \quad V(q) = \frac{1}{2} m \omega^2 q^2,$$

the scheme (5) is linearly stable. We suppose that the assumption (7) is satisfied until the end of this paragraph. The momentum p_r is defined by

$$(8) \quad p_r = \frac{\partial L_d}{\partial q_r}(q_\ell, q_r).$$

We have $p_{j+1} = m \frac{q_{j+1} - q_j}{h} - m \frac{\omega^2 h}{4} (q_{j+1} + q_j)$ and an analogous relation for p_j . Then after some lines of algebra, we obtain a discrete system involving the momentum and the state:

$$(9) \quad p_{j+1} - p_j = -m \frac{\omega^2 h}{2} (q_{j+1} + q_j), \quad \frac{q_{j+1} - q_j}{h} = \frac{1}{2m} (p_{j+1} + p_j).$$

These relations are consistent with the first order Hamilton version $\frac{dp}{dt} + m \omega^2 q = 0$, $\frac{dq}{dt} = \frac{p}{m}$ of the equations of an harmonic oscillator. Moreover, we can write the system (9) under the form

$$(10) \quad \begin{pmatrix} p_{j+1} \\ q_{j+1} \end{pmatrix} = \Phi \begin{pmatrix} p_j \\ q_j \end{pmatrix}$$

with

$$(11) \quad \Phi = \frac{1}{1 + \frac{\omega^2 h^2}{4}} \begin{pmatrix} 1 - \frac{\omega^2 h^2}{4} & -m \omega^2 h \\ \frac{h}{m} & 1 - \frac{\omega^2 h^2}{4} \end{pmatrix}.$$

Because $\det \Phi = 1$, the discrete flow (10) is symplectic as observed by Sanz-Serna [11]. Moreover, Kane *et al.* [6] have remarked that the numerical scheme (10) is one particular unconditionally stable version of the Newmark scheme [7]. Last but not least, the discrete Hamiltonian H_j defined by

$$(12) \quad H_j \equiv \frac{1}{2m} p_j^2 + \frac{m \omega^2}{2} q_j^2$$

is conserved: we have $H_{j+1} = H_j$ for $0 \leq j \leq N - 1$. We consider now a more elaborate interpolation in each interval, updating affine functions by polynomials of degree two.

3) Quadratic interpolation

Internal interpolation between 0 and h can be written in terms of quadratic finite elements [8]. For $0 \leq \theta \leq 1$, we first set

$$(13) \quad \varphi_0(\theta) = (1 - \theta)(1 - 2\theta), \quad \varphi_{1/2}(\theta) = 4\theta(1 - \theta), \quad \varphi_1(\theta) = \theta(2\theta - 1).$$

With $t = h\theta$, we consider the polynomial function

$$(14) \quad q(t) = q_\ell \varphi_0(\theta) + q_m \varphi_{1/2}(\theta) + q_r \varphi_1(\theta).$$

Then $q(0) = q_\ell$, $q(\frac{h}{2}) = q_m$ and $q(h) = q_r$ and the basis functions (13) are well adapted to these degrees of freedom. We have also

$$\begin{aligned} \frac{dq}{dt} &= \frac{1}{h} \left[q_\ell \frac{d\varphi_0}{d\theta} + q_m \frac{d\varphi_{1/2}}{d\theta} + q_r \frac{d\varphi_1}{d\theta} \right] \\ &= \frac{1}{h} \left[q_\ell (4\theta - 3) + 4q_m (1 - 2\theta) + q_r (4\theta - 1) \right] \\ &= g_\ell (1 - \theta) + g_r \theta \end{aligned}$$

with the derivatives g_ℓ and g_r given by a Gear scheme [4], *id est*

$$(15) \quad g_\ell = \frac{dq}{dt}(0) = \frac{1}{h} (-3q_\ell + 4q_m - q_r), \quad g_r = \frac{dq}{dt}(h) = \frac{1}{h} (q_\ell - 4q_m + 3q_r).$$

We remark also that

$$(16) \quad g_m = \frac{dq}{dt}\left(\frac{h}{2}\right) = \frac{1}{2}(g_\ell + g_r) = \frac{q_r - q_\ell}{h}.$$

Once the interpolation is defined in an interval of length h , we use it by splitting the range $[0, T]$ into N pieces, and $h = \frac{T}{N}$. With $t_j = jh$, we set $q_j \simeq q(t_j)$ for $0 \leq j \leq N$ and $q_{j+1/2} \simeq q(t_j + \frac{h}{2})$ with $0 \leq j \leq N-1$. In the interval $[t_j, t_{j+1}]$, the function $q(t)$ is a polynomial of degree 2, represented by the relation (14) with $t = t_j + \theta h$, $q_\ell = q_j$, $q_m = q_{j+1/2}$ and $q_r = q_{j+1}$.

4) Simpson's quadrature for a discrete Lagrangian

For the numerical integration of a regular function ψ on the interval $[0, 1]$, the midpoint method studied previously $\int_0^1 \psi(\theta) d\theta \simeq \psi(\frac{1}{2})$ is exact for a polynomial ψ of degree smaller or equal to 1. To obtain a better precision, a very popular method has been proposed by Thomas Simpson (1710-1761):

$$(17) \quad \int_0^1 \psi(\theta) d\theta \simeq \frac{1}{6} \left[\psi(0) + 4\psi\left(\frac{1}{2}\right) + \psi(1) \right].$$

The quadrature formula (17) is accurate up to polynomials of degree three. Then a discrete Lagrangian $L_h(q_\ell, q_m, q_r) \simeq \int_0^h \left[\frac{m}{2} \left(\frac{dq}{dt} \right)^2 - V(q) \right] dt$ can be defined with the Simpson quadrature formula (17) associated with an internal polynomial approximation $q(t)$ of degree 2 presented in (14):

$$(18) \quad L_h(q_\ell, q_m, q_r) = \frac{mh}{12} (g_\ell^2 + 4g_m^2 + g_r^2) - \frac{h}{6} (V(q_\ell) + 4V(q_m) + V(q_r)).$$

The discrete action Σ_d for a motion $t \mapsto q(t)$ between the initial time and a given time $T > 0$ is discretized with N regular intervals and take the form

$$(19) \quad \Sigma_d = \sum_{j=1}^{N-1} L_h(q_j, q_{j+1/2}, q_{j+1}).$$

5) Discrete Euler-Lagrange equations

We first write the Maupertuis's stationary-action principle $\delta\Sigma_d = 0$ with a variation $\delta q_{j+1/2}$ of the internal degree of freedom in the interval $[t_j, t_{j+1}]$. Due to the relations (15)(16), we first observe that $\frac{\partial g_\ell}{\partial q_m} = \frac{4}{h}$, $\frac{\partial g_m}{\partial q_m} = 0$ and $\frac{\partial g_r}{\partial q_m} = -\frac{4}{h}$. Then, due to the expression (18) of the discrete Lagrangian, we have $\frac{\partial L_h}{\partial q_m} = \frac{h}{12} \left[\frac{8m}{h} g_\ell - \frac{8m}{h} g_r - 8 \frac{dV}{dq}(q_m) \right]$. This partial derivative is equal to zero when $\delta\Sigma_d = 0$ and $m \frac{g_r - g_\ell}{h} + \frac{dV}{dq}(q_m)$ is also zero. We observe that $g_r - g_\ell = \frac{4}{h}(q_\ell - 2q_m + q_r)$ and the condition $\frac{\partial L_h}{\partial q_m} = 0$ is finally written

$$(20) \quad m \frac{4}{h^2} (q_\ell - 2q_m + q_r) + \frac{dV}{dq}(q_m) = 0.$$

We have put in evidence a second order discretization of the continuous Euler-Lagrange equation (6) of this problem. When the hypothesis (7) of an harmonic oscillator is satisfied,

we can easily solve this equation and explicit the middle value q_m as a function of the extremities:

$$(21) \quad q_m = \frac{1}{1 - \frac{\omega^2 h^2}{8}} \frac{q_\ell + q_r}{2}.$$

This interpolation is not linear if $h > 0$. This property illustrates the underlying polynomial interpolation of degree two. Moreover, a stability condition is naturally emerging:

$$(22) \quad 0 < \omega h < 2\sqrt{2}.$$

We now incorporate the relation (21) inside the expression (18) of the discrete Lagrangian. After a successful formal calculation with the help of the free software ‘‘SageMath’’ [10], we obtain a reduced Lagrangian

$$(23) \quad L_h^r(q_\ell, q_r) = \frac{1}{1 - \frac{\omega^2 h^2}{8}} \left[\frac{1}{2} m h \left(\frac{q_r - q_\ell}{h} \right)^2 - \frac{h}{2} m \omega^2 \left(\frac{22 - h^2 \omega^2}{48} (q_\ell^2 + q_r^2) + \frac{1}{12} q_\ell q_r \right) \right].$$

The discrete Euler-Lagrange (4) can now be written for this reduced Lagrangien (23). Instead of the relations (5), we obtain now the following numerical scheme:

$$(24) \quad \frac{1}{h^2} (q_{j+1} - 2q_j + q_{j-1}) + \frac{\omega^2}{24} (q_{j+1} + 22q_j + q_{j-1}) - \frac{\omega^4 h^2}{24} q_j = 0.$$

The scheme (24) is consistent with the ordinary differential equation (6)(7) $\frac{d^2 q}{dt^2} + \omega^2 q(t) = 0$. Secondly, following the definition recalled in [9], the order of truncation of the scheme (24) is obtained by replacing the discrete variables q_{j+1} , q_j and q_{j-1} by the solution of the differential equation at the precise points $t_j + h$, t_j and $t_j - h$. Then

$$\begin{cases} q_{j+1} = q_j + h \frac{dq}{dt} + \frac{h^2}{2} \frac{d^2 q}{dt^2} + \frac{h^3}{6} \frac{d^3 q}{dt^3} + \frac{h^4}{24} \frac{d^4 q}{dt^4} + \frac{h^5}{120} \frac{d^5 q}{dt^5} + \frac{h^6}{720} \frac{d^6 q}{dt^6} + O(h^7) \\ q_{j-1} = q_j - h \frac{dq}{dt} + \frac{h^2}{2} \frac{d^2 q}{dt^2} - \frac{h^3}{6} \frac{d^3 q}{dt^3} + \frac{h^4}{24} \frac{d^4 q}{dt^4} - \frac{h^5}{120} \frac{d^5 q}{dt^5} + \frac{h^6}{720} \frac{d^6 q}{dt^6} + O(h^7). \end{cases}$$

In these conditions, the left hand side of the relation (24) is no longer equal to zero and defines the truncation error $\mathcal{T}_h(q_j)$. With the help of SageMath [10], one obtains without difficulty the relation

$$\mathcal{T}_h(q_j) = \frac{1}{1440} \omega^6 h^4 q_j + O(h^6).$$

The numerical scheme (24) is fourth order accurate in the sense of the truncation error.

A fundamental question concerns stability. With the linear structure of the finite difference equation (24), we consider the equation of degree two obtained by taking $q_{j-1} = 1$, $q_j = r$ and $q_{j+1} = r^2$. The scheme is stable when the roots of the corresponding equation are of modulus smaller than 1. This equation can be written $ar^2 + br + c = 0$ with $a = 1 + \frac{h^2 \omega^2}{24}$ and $b = -\frac{1}{24} (48 - 22h^2 \omega^2 + h^4 \omega^4)$. The discriminant $\Delta \equiv b^2 - 4ac$ can be factorized:

$$\Delta = \frac{\omega^2 h^2}{576} (\omega^2 h^2 - 24) (\omega^2 h^2 - 12) (\omega^2 h^2 - 8).$$

Under the stability condition (22), all the factors in the expression of the discriminant are negative and $\Delta < 0$. Then the equation $ar^2 + br + c = 0$ has two conjugate complex roots r and \bar{r} . Their product $r\bar{r} = |r|^2$ is equal to 1 and the scheme (24) is stable.

6) Symplectic structure

From the reduced Lagrangian (23), we define the momentum p_r with the analogue of the relation (8). It comes

$$(25) \quad p_r = m \frac{q_r - q_\ell}{h} - h \frac{m \omega^2}{6} \frac{q_\ell + 2q_r}{1 - \frac{\omega^2 h^2}{8}} + h^3 \frac{m \omega^4}{48} \frac{q_r}{1 - \frac{\omega^2 h^2}{8}}.$$

This relation (25) can be explicitated in the context of grid points. We have

$$\begin{cases} p_{j+1} = m \frac{q_{j+1} - q_j}{h} - h \frac{m \omega^2}{6} \frac{q_j + 2q_{j+1}}{1 - \frac{\omega^2 h^2}{8}} + h^3 \frac{m \omega^4}{48} \frac{q_{j+1}}{1 - \frac{\omega^2 h^2}{8}} \\ p_j = m \frac{q_j - q_{j-1}}{h} - h \frac{m \omega^2}{6} \frac{q_{j-1} + 2q_j}{1 - \frac{\omega^2 h^2}{8}} + h^3 \frac{m \omega^4}{48} \frac{q_j}{1 - \frac{\omega^2 h^2}{8}}. \end{cases}$$

We eliminate the variable q_{j-1} from these two relations with the help of the difference scheme (24). We find a recurrence relation for the state $y_j \equiv (p_j, q_j)^t$, similar to the equation (10), but the matrix Φ is replaced by a matrix Φ_3 that can be explicitated:

$$(26) \quad \Phi_3 = \frac{1}{1 + \frac{\omega^2 h^2}{24}} \begin{pmatrix} 1 - \frac{11}{24} \omega^2 h^2 + \frac{\omega^4 h^4}{48} & -m \omega^2 h \left(1 - \frac{\omega^2 h^2}{12}\right) \left(1 - \frac{\omega^2 h^2}{24}\right) \\ \frac{h}{m} \left(1 - \frac{\omega^2 h^2}{8}\right) & 1 - \frac{11}{24} \omega^2 h^2 + \frac{\omega^4 h^4}{48} \end{pmatrix}.$$

We observe that the ‘‘symplectic Simpson’’ numerical scheme defined by (10)(26) is an explicit scheme. It is easy with SageMath to verify that $\det \Phi_3 = 1$ and in consequence the scheme is symplectic.

7) Conservation of a discrete energy

To explicit a discrete energy that is conserved is not *a priori* obvious. For the harmonic oscillator, we search a conserved quadratic form of the type

$$(27) \quad Q(p, q) = \frac{1}{2} \xi p^2 + \eta p q + \frac{1}{2} \zeta q^2.$$

If we require that $Q(p_{j+1}, q_{j+1}) = Q(p_j, q_j)$ with the variables p_{j+1} , q_{j+1} , p_j and q_j satisfying a linear dynamics such as (10) with a matrix

$$\Phi = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

of unit determinant, that is $\alpha \delta - \beta \gamma = 1$, then the coefficients ξ , η and ζ of the quadratic form (27) must satisfy the following homogeneous linear system

$$\Gamma \begin{pmatrix} \xi \\ \eta \\ \zeta \end{pmatrix} \equiv \begin{pmatrix} \frac{\alpha^2 - 1}{2} & \alpha \gamma & \frac{\gamma^2}{2} \\ \alpha \beta & \alpha \delta + \beta \gamma - 1 & \gamma \delta \\ \frac{\beta^2}{2} & \beta \delta & \frac{\delta^2 - 1}{2} \end{pmatrix} \begin{pmatrix} \xi \\ \eta \\ \zeta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

We have $\det \Gamma = (\alpha \delta - \beta \gamma - 1)(1 - \alpha - \delta + \alpha \delta - \beta \gamma)(1 + \alpha + \delta + \alpha \delta - \beta \gamma)$ and this expression vanishes when $\alpha \delta - \beta \gamma = 1$. Moreover, when $\alpha = \delta$, we obtain $\eta = 0$ and a conserved quadratic form Q_c can be written $Q_c(p, q) = \frac{1}{2} \gamma p^2 - \frac{1}{2} \beta q^2$ up to a multiplicative constant. Finally, if we set

$$(28) \quad H_d(p, q) \equiv \frac{1}{2m} p^2 + m \frac{\omega^2}{2 \left(1 - \frac{\omega^2 h^2}{8}\right)} \left(1 - \frac{\omega^2 h^2}{12}\right) \left(1 - \frac{\omega^2 h^2}{24}\right) q^2,$$

the symplectic Simpson scheme

$$\begin{pmatrix} p_{j+1} \\ q_{j+1} \end{pmatrix} = \Phi_3 \begin{pmatrix} p_j \\ q_j \end{pmatrix}$$

with Φ_3 explicitated at the relation (26), satisfies the following conservation of energy:

$$H_d(p_{j+1}, q_{j+1}) = H_d(p_j, q_j).$$

8) First numerical experiments

We have implemented the Simpson symplectic scheme and have compared it with the Newmark scheme (10)(11). Typical results for $N = 15$ meshes and one period are displayed on Figure 1. We have chosen $q(t) = \sin \omega t$ and $p(t) = m\omega \cos \omega t$, with a period $T = 1$. Quantitative errors with the maximum norm are presented in Table 1 below. An asymptotic order of convergence can be estimated for the momentum, the state and various energies.

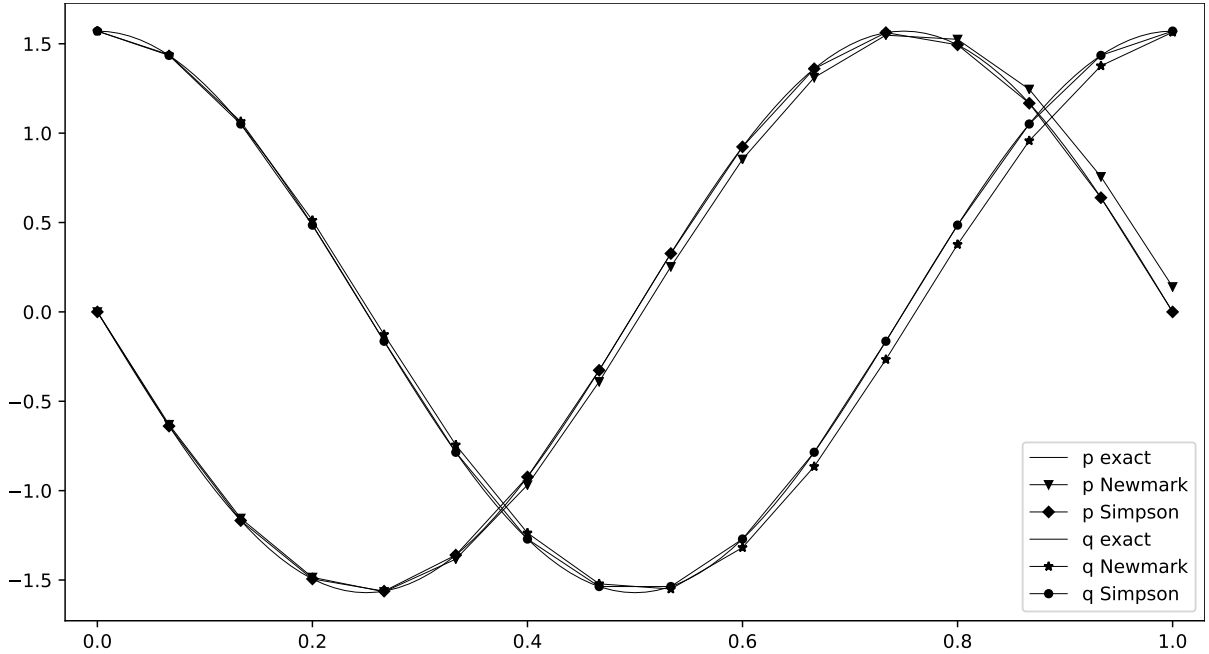


Figure 1. Typical evolution of an harmonic oscillator. The momentum p follows a cosine curve and the state q a sine shape. Comparison of the exact solution and the Newmark and symplectic Simpson schemes for $N = 15$ meshes. Both schemes give very satisfactory results. Observe that the momentum p is very close to the exact solution with the symplectic Simpson scheme. Observe that the momentum data have been rescaled.

	number of meshes	10	20	40	order
Newmark	momentum	$1.91 \cdot 10^0$	$5.02 \cdot 10^{-1}$	$1.27 \cdot 10^{-1}$	2
Symplectic Simpson	momentum	$3.41 \cdot 10^{-3}$	$2.17 \cdot 10^{-4}$	$1.35 \cdot 10^{-5}$	4
Newmark	state	$2.38 \cdot 10^{-1}$	$6.12 \cdot 10^{-2}$	$1.55 \cdot 10^{-2}$	2
Symplectic Simpson	state	$4.11 \cdot 10^{-4}$	$2.55 \cdot 10^{-5}$	$1.60 \cdot 10^{-6}$	4
Newmark	energy (12)	$1.70 \cdot 10^{-13}$	$4.97 \cdot 10^{-14}$	$1.49 \cdot 10^{-13}$	exact
Symplectic Simpson	energy (12)	$2.51 \cdot 10^{-2}$	$1.67 \cdot 10^{-3}$	$1.03 \cdot 10^{-4}$	4
Newmark	energy (28)	$2.70 \cdot 10^{-2}$	$1.67 \cdot 10^{-3}$	$1.03 \cdot 10^{-4}$	4
Symplectic Simpson	energy (28)	$2.13 \cdot 10^{-14}$	$2.49 \cdot 10^{-13}$	$1.63 \cdot 10^{-13}$	exact

Table 1. Errors in the maximum norm. We observe again that the momentum is very well approximated with the symplectic Simpson scheme. The estimated order of convergence is the closest integer α measuring the ratio of successive errors in a given line by a negative power of 2 of the type $2^{-\alpha}$.

9) Conclusion and perspectives

The symplectic Simpson numerical scheme has been developed in this contribution. It has been tested for an harmonic oscillator. The method is symplectic, conditionnally stable and is fourth order accurate for state and momentum.

An important question is still open concerning the nonlinear case. The elimination of the internal degree of freedom is not possible in that case. Once this question has a satisfactory answer, the extension to systems with mutiple degrees of freedom is a natural objective for future studies.

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