Volume-energy preserving integrators for piecewise smooth approximations of Hamiltonian systems

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Abstract

In this paper, we consider Hamiltonian systems obtained from a $C^{1,1}$ approximation of the Hamiltonian function: we prove the existence of a first derivative of the flow with respect to initial values and show that it satisfies the symplecticity condition almost everywhere in the phase-space. In a second step, we address the construction of such an approximation through B-splines and we apply a splitting method introduced by R. McLachlan and R. Quispel [9] to the resulting *discrete* system. Eventually, we prove that the combined numerical method is of order 2, is sympletic, and preserves the original energy up to an error of a magnitude prescribed by the user and resulting from the B-splines approximation.

Keywords: Hamiltonian systems, symplecticity, volume-preservation, energy-preservation, B-splines, weak order.

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1 Introduction

Consider a Hamiltonian system

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H(q,p), \\ \dot{p} & = & -\nabla_q H(q,p), \end{array} \right. \tag{1.1}$$

where $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$, and with a separable Hamiltonian H of the form

$$H(q,p) = \frac{1}{2} p^T p + V(q), \tag{1.2}$$

where $V(q)$ is the potential function. In many applications, such as for instance molecular dynamics, it is of importance that the numerical flow used to compute the solution of (1.1) preserves the volume form and the Hamiltonian. However, it is generally admitted that no standard method can satisfy both requirements, apart from exceptional situations such as for instance a quadratic Hamiltonian[1]. A possible approach could be to solve in sequence the d

[1]For B-series methods, volume preservation implies symplecticity [3]; since the only symplectic and Hamiltonian-preserving B-series method is the exact flow [2], this shows that there exists no B-series method preserving both the energy and the volume.

Hamiltonian systems with Hamiltonians

$$H^{[i]}(q_i, p_i) = \frac{1}{2}p_i^2 + V^{[i]}(q_i) + \frac{1}{2}\sum_{j\neq i} \bar{p}_j^T \bar{p}_j, \tag{1.3}$$

$$V^{[i]}(q_i) = V\left(\bar{q}_1, \ldots, \bar{q}_{i-1}, q_i, \bar{q}_{i+1}, \ldots, \bar{q}_d\right), \tag{1.4}$$

obtained by freezing all components (denoted with a bar) except the two conjugate coordinates q_i and p_i. If each subsystem can be solved exactly and the same step-size is used for all, the resulting "numerical" method preserves the desired quantities, since each sub-step is symplectic and preserves $H^{[i]}$ (and thus H). Considering that each subsystem is of dimension 2 and thus integrable, it can be hoped that an exact solution is indeed obtainable in some specific situations. Nevertheless, such situations are rather non-generic, though it is important to mention at this stage the special case of *multi-quadratic* potentials, i.e. potentials such that for all $i = 1, \ldots, d$ and all $q \in \mathbb{R}^d$, $V^{[i]}$ is *quadratic* in q_i. In this context, the method described above[2] has been introduced in by R. Quispel and R.I. McLachlan in [9].

In order to retain the possibility of solving exactly each sub-system and at the same time to cover more general problems, we give up the requirement of exact Hamiltonian preservation and we consider a multi-quadratic piecewise approximation of H. If instead of (1.1) we now solve

$$\left\{ \begin{array}{rcl} \dot{q} &=& \nabla_p H^\tau(q,p), \\ \dot{p} &=& -\nabla_q H^\tau(q,p), \end{array} \right. \tag{1.5}$$

where $H^\tau(q,p) = \frac{1}{2}p^T p + V^\tau(q)$ is a $C^{1,1}$ multi-quadratic approximation of H, the aforementioned procedure applied with exact solution of the sub-systems gives a first-order method which preserves H^τ exactly as well as the volume form. If $\sup_K |H - H^\tau| \leq C_K\ \tau^2$ for a compact subset K of $\mathbb{R}^d \times \mathbb{R}^d$ containing the numerical solution, then H is conserved up to an error of size $\mathcal{O}(\tau^2)$ over arbitrarily long intervals of integration (including infinite ones).

Note that this approach remains valid for more general Hamiltonians (non-separable for instance), provided an exact solution can be computed, so that all theoretical results concerning the conservation of energy and volume will be stated for general Hamiltonians. In contrast, we will describe the implementation of the method with quadratic B-splines only for the case of separable Hamiltonians.

In Section 2, we prove the main properties of the flow of Hamiltonian systems with globally Lipschiz derivative: in particular, we show that the exact flow remains symplectic, volume preserving and Hamiltonian preserving, though in a weaker sense. We also prove the existence of a Taylor expansion in the sense of distribution and establish the order of a general composition of flows for split systems. Section 3 is devoted to B-splines approximation of separable Hamiltonians in the one-dimensional case ($(q,p) \in \mathbb{R}^2$): an explicit expression of the exact solution is given that will serve as a basis for higher dimensions. Section 4 is concerned with B-splines approximation for the d-dimensional case and the numerical scheme used here is shown to be of order 1 and becomes an order 2 method when composed with its adjoint, though in a slightly weaker sense than usual. Section 5 presents numerical results for three different test problems, for which the usual behaviour of symplectic integrators is exhibited.

[2] It is worth mentioning that for multi-quadratic Hamiltonians, there is an alternative to the exact solution of each sub-step: the implicit midpoint rule is both Hamiltonian and volume preserving (as would be indeed any non-partitioned symplectic method), and turns out to be explicit owing to the linearity of the vector fields [9].

2 Hamiltonians systems with non-differentiable vector fields

We consider Hamiltonian functions H that are $\mathcal{C}^{1,1}$ over the whole phase space $\mathbb{R}^{2d}$. Under this assumption, the function $y \mapsto \nabla H(y)$ is continuous on $\mathbb{R}^{2d}$ and Lipschitz[3]. This ensures the existence and uniqueness of the solution of the associated Hamiltonian system:

$$\forall\, t \in \mathbb{R}, \quad \frac{\mathrm{d}y}{\mathrm{d}t}(t) = J^{-1}\nabla H\left(y(t)\right), \quad y(0) = y_0 \in \mathbb{R}^{2d} \tag{2.1}$$

where J is the constant matrix

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Our aim in this section is to show that under these assumptions on the regularity of H, the flow φ_t associated with the differential system (2.1) is weakly symplectic and weakly volume-preserving, i.e. that the usual matrix equalities hold almost everywhere (a.e.) on $\mathbb{R}^{2d}$ for the Lebesgue measure. In the sequel, we will use the notations

$$\begin{aligned} \langle f|g\rangle &= \int_{\mathbb{R}^{2d}} g^T(y) f(y) dy = \int_{\mathbb{R}^{2d}} g^T f, \\ \langle f|M|g\rangle &= \int_{\mathbb{R}^{2d}} g^T(y) M(y) f(y) dy = \int_{\mathbb{R}^{2d}} g^T M f, \end{aligned}$$

for all functions $f(y)$ and $g(y)$ from $\mathbb{R}^{2d}$ to itself and all linear mappings $M(y)$ from $\mathbb{R}^{2d}$ to itself, for which the expression is well-defined.

Lemma 2.1 *Let f be a Lipschitz function from $\mathbb{R}^{2d}$ to itself. Then f is a.e. differentiable, i.e. for a.e. $y \in \mathbb{R}^{2d}$ there exists a linear mapping $f'(y)$ from $\mathbb{R}^{2d}$ to $\mathbb{R}^{2d}$ such that*

$$f(y + \Delta y) = f(y) + f'(y)\Delta y + o(\|\Delta y\|) \text{ as } \|\Delta y\| \to 0.$$

Moreover, f' coincide with its derivative in the sense of distributions, i.e. for all Lipschitz functions g from $\mathbb{R}^{2d}$ to itself with compact support, we have

$$-\int_{\mathbb{R}^{2d}} g^T f' = \int_{\mathbb{R}^{2d}} f^T g'. \tag{2.2}$$

Proof. The existence of a derivative $f'(y)$ for a.e. $y \in \mathbb{R}^{2d}$ is stated in Rademacher's Theorem (see for instance [5] pp. 81). Although (2.2) is totally standard in functional analysis, we present here a short proof for the convenience of the reader: for a fixed unit-vector η, the sequence of functions

$$f_n(y) = \frac{f(y + \frac{1}{n}\eta) - f(y)}{\frac{1}{n}}$$

converges towards $f'(y)\eta$ a.e on $\mathbb{R}^{2d}$ and is uniformly bounded by L:

$$\|f_n(y)\| \leq n\|f(y + \frac{1}{n}\eta) - f(y)\| \leq nL\frac{1}{n} \leq L.$$

[3]We could also assume that H is locally $\mathcal{C}^{1,1}$ which would yield local existence and uniqueness results.

Given a test function g globally Lipschitz on $\mathbb{R}^{2d}$, the equality

$$\int_{\mathbb{R}^{2d}} \left(\frac{g(y+\frac{1}{n}\eta)-g(y)}{\frac{1}{n}} \right)^T f(y)dy = -\int_{\mathbb{R}^{2d}} g^T(y) \left(\frac{f(y)-f(y-\frac{1}{n}\eta))}{\frac{1}{n}} \right) dy$$

and the Dominated Convergence Theorem imply

$$\int_{\mathbb{R}^{2d}} f^T g'\eta = -\int_{\mathbb{R}^{2d}} g^T f'\eta.$$

■

Theorem 2.2 *Let H be a continuously differentiable scalar function defined on $\mathbb{R}^{2d}$ such that $f = J^{-1}\nabla H$ is Lipschitz over the whole space $\mathbb{R}^{2d}$ and consider the flow φ_t associated with f. Then, for a fixed $t \in \mathbb{R}$, φ_t satisfies the following properties:*

- *(i) φ_t is continuous and globally Lipschitz.*
- *(ii) φ_t is one-to-one and $\varphi_t^{-1} = \varphi_{-t}$.*
- *(iii) for any $y \in \mathbb{R}^{2d}$, $H(\varphi_t(y)) = H(y)$, that is to say φ_t is Hamiltonian-preserving.*
- *(iv) φ_t is a.e. differentiable on $\mathbb{R}^{2d}$.*
- *(v) ∇H is a.e. differentiable on $\mathbb{R}^{2d}$ and its derivative $\nabla^2 H$ is symmetric a.e.*
- *(vi) $(\varphi_t')^T J \varphi_t' = J$ a.e. on $\mathbb{R}^{2d}$.*
- *(vii) $|det(\varphi_t')| = 1$ a.e. on $\mathbb{R}^{2d}$.*

Proof. The vector field being Lipschitz-continuous on $\mathbb{R}^{2d}$, (i), (ii) and (iii) follow at once from standard theorems.

(iv) is a a consequence of Lemma 2.1. Similarly, $f = J^{-1}\nabla H$, φ_s and $f \circ \varphi_s$ are differentiable a.e. Besides, φ_s has a Lipschitz inverse so that

$$(f \circ \varphi_s)' = f' \circ \varphi_s \cdot \varphi_s' \text{ a.e. on } \mathbb{R}^{2d}.$$

Though it seems familiar, this relation is far from being obvious and requires in essence that the function φ_s does not contract sets of non-zero measure to negligible ones. We refer the reader to [5] pp. 85 for a proof of a very similar result and also to [4] and [1] for a situation where much less regularity on f and φ_s is required.

(v) is a consequence of the relation

$$\int_{\mathbb{R}^{2d}} \partial_j(\partial_i H)\cdot G = -\int_{\mathbb{R}^{2d}} (\partial_i H)\cdot(\partial_j G) = \int_{\mathbb{R}^{2d}} H\cdot(\partial_j\partial_i G) = \int_{\mathbb{R}^{2d}} \partial_i(\partial_j H)\cdot G,$$

valid for smooth scalar functions G.

In order to prove (vi), let us consider a smooth g and a fixed vector η. The function $\langle \eta|\varphi_t'|g\rangle$ is differentiable with respect to t and

$$\frac{d}{ds}\langle \eta|\varphi_s'|g\rangle \;=\; -\int_{\mathbb{R}^{2d}} (\dot{\varphi}_s)^T g'\eta = -\int_{\mathbb{R}^{2d}} (f\circ\varphi_s)^T g'\eta = \langle \eta|(f\circ\varphi_s)'|g\rangle. \qquad (2.3)$$

Consider now $g \in L^1(\mathbb{R}^{2d};\mathbb{R}^{2d})$ with compact support K and g_n a sequence of smooth functions such that $g_n \to g$ in $L^1(K;\mathbb{R}^{2d})$. For all $s \in (-t,t)$ and for a.e. $x \in K$, the functions φ_s' and $(f\circ\varphi_s)'$ are bounded, so that the sequences of continuous functions $\langle\varphi_s'|g_n\rangle$ and $\langle(f\circ\varphi_s)'|g_n\rangle$ converge uniformly on $(-t,t)$ toward $\langle\varphi_s'|g\rangle$ and $\langle(f\circ\varphi_s)'|g\rangle$. This shows that

$$\frac{d}{ds}\langle\eta|\varphi_s'|g\rangle = \frac{d}{ds}\lim_{n\to\infty}\langle\eta|\varphi_s'|g_n\rangle = \lim_{n\to\infty}\langle\eta|(f\circ\varphi_s)'|g_n\rangle = \langle\eta|(f\circ\varphi_s)'|g\rangle,$$

i.e. that (2.3) is also valid for test functions in $L^1(\mathbb{R}^{2d};\mathbb{R}^{2d})$ with compact support. Hence, given any two Lipschitz functions g_1 and g_2 with compact supports we have

$$\frac{d}{ds}\langle g_1|\varphi_s'|g_2\rangle \;=\; \frac{d}{ds}\int_{\mathbb{R}^{2d}} g_1^T\varphi_s' g_2 = \int_{\mathbb{R}^{2d}} g_1^T(f\circ\varphi_s)' g_2 = \langle g_1|f'\circ\varphi_s\cdot\varphi_s'|g_2\rangle, \quad (2.4)$$

so that the function $G(u,v)=\langle g_1|(\varphi_u')^T J\varphi_v'|g_2\rangle$ is well defined for u and v in $(-t,t)$ and has continuous partial derivatives given by

$$\partial_u G(u,v) = \langle g_1|(\varphi_u')^T(f'\circ\varphi_u)^T J\varphi_v'|g_2\rangle \text{ and } \partial_v G(u,v) = \langle g_1|(\varphi_u')^T J(f'\circ\varphi_v)\varphi_v'|g_2\rangle.$$

As a consequence $G(s,s)$ is continuously differentiable and

$$\frac{d}{ds}G(s,s) = \partial_u G(s,s) + \partial_v G(s,s) = \int_{\mathbb{R}^{2d}} g_1^T(\varphi_s')^T\Big((f'(\varphi_s))^T J - Jf'(\varphi_s)\Big)\varphi_s' g_2,$$

hence $\partial_s G(s,s)=0$ owing to point (v). This completes the proof of (vi). Eventually, (vii) is an easy consequence of (vi). ∎

Theorem 2.3 *Let H be a continuously differentiable scalar function defined on $\mathbb{R}^{2d}$ such that $f = J^{-1}\nabla H$ is Lipschitz over the whole space $\mathbb{R}^{2d}$ and consider the flow φ_t associated with f. For any $t\in\mathbb{R}$ and any measurable set K of $\mathbb{R}^{2d}$, we have*

$$\int_K dy = \int_{\varphi_t(K)} dy. \quad (2.5)$$

Besides, if K is a compact set of $\mathbb{R}^2$ and ψ a diffeomorphism from K to $\mathbb{R}^{2d}$, then we have

$$\int_K \left(\frac{\partial(\varphi_t\circ\psi)}{\partial u}(u,v)\right)^T J\frac{\partial(\varphi_t\circ\psi)}{\partial u}(u,v)dudv = \int_K \left(\frac{\partial\psi}{\partial u}(u,v)\right)^T J\frac{\partial\psi}{\partial u}(u,v)dudv. \quad (2.6)$$

Proof. In order to get some insight of the result, we first give an elementary and intuitive proof of (2.5) for compact sets of the form

$$K_{\eta,c} = \{y\in\mathbb{R}^{2d},\ \|y-c\|_\infty \le \frac{\eta}{2}\},\ \eta>0 \text{ and } c\in\mathbb{R}^{2d}.$$

Consider φ_t^ε the flow of the system with Hamiltonian $H^\varepsilon = \rho^\varepsilon \star H$ where ρ^ε is a mollifier and where star denotes the convolution product. For all $t\in\mathbb{R}$, φ_t^ε is a volume-preserving diffeomorphism of $\mathbb{R}^{2d}$, so that (2.5) is trivially satisfied for φ_t^ε. Now, for a fixed $t\in\mathbb{R}$, Gronwall's lemma shows that there exists a constant $\nu(t)$ such that

$$\sup_{y\in\mathbb{R}^{2d}} \|\varphi_t^\varepsilon(y)-\varphi_t(y)\|_\infty \le \nu(t)\varepsilon.$$

Now, consider $y\in\varphi_t(K_{\eta,c})$: we have

$$\|\varphi_{-t}(y)-c\|_\infty \le \frac{\eta}{2} \Longrightarrow \|\varphi_{-t}^\varepsilon(y)-c\|_\infty \le \frac{\eta}{2}+\nu(t)\varepsilon \Longrightarrow y\in\varphi_t^\varepsilon(K_{\eta+2\nu(t)\varepsilon}).$$

Symmetrically, for a small enough ε, consider $y \in \varphi_t^\varepsilon(K_{\eta-2\nu(t)\varepsilon,c})$: we have

$$\|\varphi_{-t}^\varepsilon(y) - c\|_\infty \leq \frac{\eta}{2} - \nu(t)\varepsilon \Longrightarrow \|\varphi_{-t}(y) - c\|_\infty \leq \frac{\eta}{2} \Longrightarrow y \in \varphi_t(K_{\eta,c}).$$

Summing up, we obtain

$$\varphi_t^\varepsilon(K_{\eta-2\nu(t)\varepsilon,c}) \subset \varphi_t(K_{\eta,c}) \subset \varphi_t^\varepsilon(K_{\eta+2\nu(t)\varepsilon,c}),$$

and as a direct consequence

$$(\eta - 2\nu(t)\varepsilon)^{2d} = \int_{\varphi_t^\varepsilon(K_{\eta-2\nu(t)\varepsilon,c})} dy \leq \int_{\varphi_t(K_{\eta,c})} dy \leq \int_{\varphi_t^\varepsilon(K_{\eta+2\nu(t)\varepsilon,c})} dy = (\eta + 2\nu(t)\varepsilon)^{2d}.$$

We get (2.5) in the limit $\varepsilon \to 0$.

For the general case of a measurable set K, (2.5) is a consequence of the area formula, which is valid for all Lipschitz functions (see for instance Theorem 1 of [5] pp.96)

$$\int_{\varphi_t(K)} dy = \int_K |\varphi'_{-t}(y)| dy, \tag{2.7}$$

and of point (vii) of Theorem 2.2 applied to $\varphi_{-t} = \varphi_t^{-1}$.

Relation (2.6) is a consequence of point (vi) of Theorem 2.2 and of the chain rule for $\varphi_t \circ \psi$ which holds in this case owing to the fact that φ_t, ψ and ψ^{-1} are Lipschitz functions. ■

Lemma 2.4 *Let f and Γ be two Lipschitz functions from $\mathbb{R}^{2d}$ to itself and consider the flow φ_s associated with f. If div$(f) = 0$ a.e., then, for any Lipschitz g with compact support K, the function $\langle \Gamma \circ \varphi_s | g \rangle$ is continuously differentiable on $(-t, t)$ and we have for $-t < s < t$:*

$$\frac{d}{ds}\langle \Gamma \circ \varphi_s | g \rangle = \langle (\Gamma \circ \varphi_s)' f | g \rangle = \langle (\Gamma' \circ \varphi_s)\varphi'_s f | g \rangle \tag{2.8}$$

Moreover, the following Taylor expansion holds:

$$\langle \Gamma \circ \varphi_s | g \rangle = \langle \Gamma | g \rangle + s\langle \Gamma' f | g \rangle + \mathcal{O}\left(s^2 \, L_\Gamma \, \|g'\|_{L^1} \, \|f\|^2_{L^\infty(K)} \right), \tag{2.9}$$

where L_Γ is the Lipschitz constants of Γ, $\|\cdot\|_{L^1}$ is the L^1-norm on $\mathbb{R}^{2d}$ and where the constant in the term $\mathcal{O}$ depends on t.

Proof. Let us suppose that $g = (g^1, \ldots, g^{2d})^T$ where all g_i's are smooth functions from $\mathbb{R}^{2d}$ to $\mathbb{R}$. Then, upon using a change of variables formula (see Theorem 2 of [5] pp. 99) with $|\varphi'_s| = 1$, we have

$$\langle \Gamma \circ \varphi_s | g \rangle = \int_{\mathbb{R}^{2d}} \Gamma^T (g \circ \varphi_{-s})$$

from which we see that $\langle \Gamma \circ \varphi_s | g \rangle$ is C^1 on $(-t, t)$ and that

$$\frac{d}{ds}\langle \Gamma \circ \varphi_s | g \rangle \;\; = \;\; -\int_{\mathbb{R}^{2d}} \Gamma^T (g' \circ \varphi_{-s})(f \circ \varphi_{-s}).$$

Going back to previous variables, it follows that

$$\frac{d}{ds}\langle \Gamma \circ \varphi_s | g \rangle = -\int_{\mathbb{R}^{2d}} (\Gamma \circ \varphi_s)^T g' f = \int_{\mathbb{R}^{2d}} g^T (\Gamma \circ \varphi_s)' f$$

owing to the fact that $\sum_k (\partial_k f^k) = \text{div}(f) = 0$ a.e. [4] We can now prove (2.9) for Lipschitz functions by a density argument just as in the proof of point (vi) in Theorem 2.2. Eventually, since $\langle \Gamma \circ \varphi_s, g \rangle$ is continuously differentiable on $(-t, t)$, estimate (2.9) follows straightforwardly from the bound

$$|\langle (\Gamma \circ \varphi_s)' f | g \rangle - \langle \Gamma' f | g \rangle| \leq |\langle \Gamma \circ \varphi_s - \Gamma | g' f \rangle| \leq s\, C\, L_\Gamma\, \|g'\|_{L^1}\, \|f\|^2_{L^\infty(K)},$$

where L_Γ is the Lipschitz constant of Γ and where C is a constant depending on t. ∎

Lemma 2.5 *Consider n vector fields $f_1, f_2, \ldots, f_n$ where the f_i's are Lipschitz functions from $\mathbb{R}^{2d}$ to itself satisfying div$(f_i) = 0$ a.e., and for all $i = 1, \ldots, n$ let $\varphi_{i,u}$ be the flow associated with f_i. Then, for all Lipschitz functions g with compact support K and for u and v in $(-t, t)$, the following weak Taylor Lagrange expansions hold:*

$$\begin{aligned} \langle \varphi_{u_1,1} \circ \ldots \circ \varphi_{u_n,n} | g \rangle &= \langle y + \sum_i u_i f_i + \sum_{i<j} u_i u_j f_i' f_j + \sum_i \frac{u_i^2}{2} f_i' f_i | g \rangle \\ &\quad + \sum_{i \leq j} \mathcal{O}\left(\|g'\|_{L^1}\, u_i^2 u_j \right), \end{aligned} \tag{2.10}$$

where the constant in the term $\mathcal{O}$ depends on the L_{f_i}'s, on the $\|f_j\|_{L^\infty(K)}$'s and on t.

Proof. We first prove the estimate for one vector field f and the corresponding flow φ_u: define $\theta(u) = \langle \varphi_u | g \rangle$. Using formula (2.8), first with $\Gamma(y) = y$ and then with $\Gamma(y) = f(y)$, we straightforwardly obtain $\dot\theta(u) = \langle f \circ \varphi_u | g \rangle$ and $\ddot\theta(u) = \langle (f \circ \varphi_u)' f | g \rangle$. Estimate (2.9) then leads to

$$|\theta(u) - \theta(0) - u\dot\theta(0) - \frac{u^2}{2}\ddot\theta(0)| \leq \frac{u^3}{6}\, C\, L_f\, \|g'\|_{L^1}\, \|f\|^2_{L^\infty(K)}. \tag{2.11}$$

We thus obtain (2.10) for $n = 1$ by noticing that $\ddot\theta(0) = \langle f, g \rangle$ and $\ddot\theta(0) = \langle f' f | g \rangle$.

Consider now the function $\theta(u, v) = \langle \varphi_{u,1} \circ \varphi_{v,2} | g \rangle$. Noticing that $\theta(u, v) = \langle \varphi_{u,1} | g \circ \varphi_{-v,2} \rangle$, we have

$$\begin{aligned} \theta(u,v) &= \langle y + u f_1 + \frac{u^2}{2} f_1' f_1 | g \circ \varphi_{-v,2} \rangle + \mathcal{O}(u^3), \\ &= \langle \varphi_{v,2} | g \rangle + u \langle f_1 \circ \varphi_{v,2} | g \rangle + \frac{u^2}{2} \langle f_1' \circ \varphi_{v,2} \cdot f_1 \circ \varphi_{v,2} | g \rangle + \mathcal{O}(u^3), \\ &= \langle y + v f_2 + \frac{v^2}{2} f_2' f_2 | g \rangle + u \langle f_1 | g \rangle + uv \langle f_1' f_2 | g \rangle + \frac{u^2}{2} \langle f_1' f_1 | g \rangle \\ &\quad + \mathcal{O}(u^3) + \mathcal{O}(v^3) + \mathcal{O}(u^2 v) + \mathcal{O}(u v^2). \end{aligned}$$

This proves (2.10) for $n = 2$. The general case follows by induction. ∎

[4] Note that if Γ is continuously differentiable, the same equality can be obtained straightforwardly, in particular without using the change of variable formula.

Corollary 2.6 *Consider a split vector field $f = f_1 + \dots f_n$ where the f_i's are Lipschitz functions from $\mathbb{R}^{2d}$ to itself satisfying div$(f_i) = 0$ a.e., and for all $i = 1, \dots, n$ let $\varphi_{u,i}$ be the flow associated with f_i, and φ_t the flow associated with f. Then, for all Lipschitz functions g with compact support K and for s in $(-t, t)$, the following weak Taylor Lagrange expansions hold for $\Phi_s = \varphi_{s,1} \circ \dots \circ \varphi_{s,n}$*

$$\langle \Phi_s | g \rangle = \langle \varphi_s | g \rangle + \mathcal{O}(s^2 \|g\|_{L^1}), \tag{2.12}$$

that is to say the Φ_s is of (strong) order 1, and

$$\langle \Phi_{s/2} \circ \Phi_{s/2}^* | g \rangle = \langle \varphi_s | g \rangle + \mathcal{O}(s^3 \|g'\|_{L^1}), \tag{2.13}$$

that is to say the $\Phi_{s/2} \circ \Phi_{s/2}^*$ is of (weak) order 2.

Proof. Equation (2.12) is obtained as in Lemma 2.5. The strong order follows from a density argument. We prove the weak order 2 by applying previous lemma with $f = \frac{1}{2} f_1 + \dots \frac{1}{2} f_n + \frac{1}{2} f_n + \dots \frac{1}{2} f_1$, $u_1 = u_2 = \dots = u_{2n} = s/2$ and comparing the different terms with those of the development of $\langle \varphi_s | g \rangle$. ■

3 One degree of freedom example

In this section, we consider the case of a Hamiltonian of the form

$$H(q, p) = \frac{p^2}{2} + V(q)$$

where $p \in \mathbb{R}$ and $V : \mathbb{R} \mapsto \mathbb{R}$ is a potential function.

3.1 Approximation using quadratic B-splines functions

Let τ be a real number, and let V_n be the values of the potential V at the grid points $(n+1/2)\tau$, $n \in \mathbb{Z}$. We define the interpolant $V^\tau(q)$ of $V(q)$ as the function

$$V^\tau(q) := \sum_{n \in \mathbb{Z}} V_n \, B_n(q) \tag{3.1}$$

where $B_n(q)$ is the B-splines function of order 3 defined by

$$B_n(q) = \begin{cases} \frac{1}{2} \left(\frac{q - (n-1)\tau}{\tau} \right)^2, & (n-1)\tau \le q \le n\tau, \\ -\left(\frac{q - n\tau}{\tau} \right)^2 + \left(\frac{q - n\tau}{\tau} \right) + \frac{1}{2}, & n\tau \le q \le (n+1)\tau, \\ \frac{1}{2} \left(\frac{(n+2)\tau - q}{\tau} \right)^2, & (n+1)\tau \le q \le (n+2)\tau, \\ 0, & \textit{elsewhere}. \end{cases} \tag{3.2}$$

The function (3.1) is a $\mathcal{C}^1$ real function over $\mathbb{R}$, and is piecewise quadratic with respect to the decomposition $\mathbb{R} = \bigsqcup_{n\in\mathbb{Z}} [n\tau, (n+1)\tau]$. The corresponding Hamiltonian $H^\tau(q,p) = \frac{1}{2}p^2 + V^\tau(q)$ is then piecewise quadratic with respect to the decomposition

$$\mathbb{R}^2 = \bigsqcup_{n\in\mathbb{Z}} [n\tau, (n+1)\tau] \times \mathbb{R}.$$

The following approximation result shows that if V is $\mathcal{C}^2$, the function $V^\tau(q)$ is a $\mathcal{C}^1$ approximation of V on all compact subsets of $\mathbb{R}$:

Proposition 3.1 *Assume that V is a $\mathcal{C}^2$ function on $\mathbb{R}$ such that $\nabla^2 V$ is bounded on $\mathbb{R}$. The function V^τ defined above satisfies the estimates:*

$$\max_{q\in\mathbb{R}} |V(q) - V^\tau(q)| \leq C_1\tau^2 \quad \textit{and} \quad \max_{q\in\mathbb{R}} |\nabla V(q) - \nabla V^\tau(q)| \leq C_2\tau \tag{3.3}$$

where the constants C_1 and C_2 depend only on $\max_{q\in\mathbb{R}} |\nabla^2 V(q)|$.

Moreover, for a given $\tau_0 > 0$, the function $V^\tau(q)$ is uniformly $\mathcal{C}^{1,1}$ on $\mathbb{R}$ for $\tau \in (0, \tau_0)$.

Proof. Let $n\tau \leq q \leq (n+1)\tau$. Denoting $x = \frac{q-n\tau}{\tau}$, we have

$$V^\tau(q) = \frac{1}{2}V_{n-1}\,(1-x)^2 + V_n\left(-x^2 + x + \frac{1}{2}\right) + \frac{1}{2}V_{n+1}x^2,$$

that is to say

$$V^\tau(q) = \frac{1}{2}(V_n + V_{n-1}) + x(V_n - V_{n-1}) + \frac{1}{2}x^2(V_{n+1} - 2V_n + V_{n-1}). \tag{3.4}$$

Using Taylor expansions, we obtain

$$\begin{aligned} V_{n-1} &= V(q) + \tau(-\tfrac{1}{2} - x)\nabla V(q) + \mathcal{O}(\tau^2), \\ V_n &= V(q) + \tau(\tfrac{1}{2} - x)\nabla V(q) + \mathcal{O}(\tau^2), \\ V_{n+1} &= V(q) + \tau(\tfrac{3}{2} - x)\nabla V(q) + \mathcal{O}(\tau^2). \end{aligned}$$

where the terms in $\mathcal{O}(\tau^2)$ depend on $\max_{(n-1)\tau\leq q\leq(n+1)\tau} |\nabla^2 V(q)|$. Plugging these expressions into (3.4), we get

$$V^\tau(q) = V(q) + \mathcal{O}(\tau^2).$$

Similarly, using $\partial_q = \tau^{-1}\partial_x$, we have

$$\nabla V^\tau(q) = \frac{1}{\tau}(V_n - V_{n-1}) + \frac{1}{\tau}x(V_{n+1} - 2V_n + V_{n-1}) = \nabla V(q) + \mathcal{O}(\tau). \tag{3.5}$$

This completes the proof of (3.3). Moreover, using (3.5) it is easy to show that there exists a numerical constant C_3 such that we have

$$\forall\, q_1, q_2 \in \mathbb{R}, \quad |\nabla V^\tau(q_1) - \nabla V^\tau(q_2)| \leq (1 + C_3\tau)\left(\max_{q\in\mathbb{R}} |\nabla^2 V(q)|\right) |q_1 - q_2|$$

and this shows that the function $V^\tau(q)$ uniformly $\mathcal{C}^{1,1}$ on $\mathbb{R}$ for sufficiently small τ. ∎

The following approximation result is an easy application of the previous proposition:

Theorem 3.2 *Let φ_t be the flow of the Hamiltonian system with Hamiltonian H and φ_t^τ be the flow of the Hamiltonian system with Hamiltonian H^τ. Let us fix $\tau_0 > 0$. Then we have the estimate:*

$$\forall\, 0 < \tau \leq \tau_0,\ \forall\, y \in \mathbb{R}^2,\ \forall\, T > 0,\ \|\varphi_T(y) - \varphi_T^\tau(y)\| \leq \frac{C_2 \tau}{L} \left(\exp(LT) - 1\right), \tag{3.6}$$

where L is the Lipschitz constant of ∇V.

3.2 Integration of the system

The aim of this subsection is to give an explicit expression of the exact solution of the Hamiltonian system

$$\left\{ \begin{array}{rcl} \dot{q}(t) & = & p(t), \\ \dot{p}(t) & = & -\nabla V^\tau(q(t)). \end{array} \right. \tag{3.7}$$

Let $n = E[q(0)/\tau]$. The solution of (3.7) in $[n\tau, (n+1)\tau] \times \mathbb{R}$ is given by the system

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \beta_n & 0 \end{pmatrix} \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} + \begin{pmatrix} 0 \\ \alpha_n \end{pmatrix} \tag{3.8}$$

where

$$\alpha_n = \frac{1}{\tau}\left(V_{n-1} - V_n + n(V_{n+1} - 2V_n + V_{n-1})\right) \quad \text{and} \quad \beta_n = -\frac{1}{\tau^2}(V_{n+1} - 2V_n + V_{n-1}).$$

Its exact solution can be written explicitly as

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = e^{A_n t} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} + \int_0^t e^{A_n(t-s)} \begin{pmatrix} 0 \\ \alpha_n \end{pmatrix} ds \tag{3.9}$$

where

$$A_n = \begin{pmatrix} 0 & 1 \\ \beta_n & 0 \end{pmatrix}.$$

Formula (3.9) remains valid as long as $q(t)$ stays in $[n\tau, (n+1)\tau]$.

Another way of computing the (geometric) trajectories is as follows: suppose that $H_0 = \frac{1}{2}p_0^2 + V^\tau(q_0)$ is given. In a domain $K_n = [n\tau, (n+1)\tau] \times \mathbb{R}$, the trajectory corresponds to the set

$$\{(q,p) \in K_n \mid \tfrac{1}{2}p^2 - \tfrac{1}{2}\alpha_n q^2 - \beta_n q + \delta_n = H_0\} \tag{3.10}$$

where

$$\delta_n = \frac{1}{2}(V_n + V_{n-1}) - n(V_n - V_{n-1}) + \frac{1}{2}n^2(V_{n+1} - 2V_n + V_{n-1}).$$

The set (3.8) is simply the intersection of K_j with a conic. Hence, the trajectory is a piecewise conic curve.

Starting from $(q_0, p_0) \in \mathbb{R}^2$, an algorithm to integrate exactly (3.7) can be written as follows:

1. Determine $n_0 = E(q_0/\tau)$

2. Compute the solution (3.9) in K_{n_0} and solve for $t_1 > 0$ such that $q(t_1) = (n_0 + 1)\tau$. If there is a solution, let $p_1 = p(t_1)$, $q_1 = (n_0+1)\tau$, $n_1 = n_0+1$, and continue to integrate in K_{n_1} (if there are more than one positive solution, take the minimum).

3. If there is no solution to Step 2, solve for $t_1 > 0$ such that $q(t_1) = n_0\tau$ and $p(t_1) \neq p(0)$. If there is a solution, let $p_1 = p(t_1)$, $q_1 = n_0\tau$, $n_1 = n_0 - 1$, and continue to integrate in K_{n_1}.

4. If there is no solution to (3), let $n_1 = n_0 - 1$, and continue to integrate in K_{n_1}.

This procedure can be repeated until a given time t. The algorithm is described with full details in the Appendix section.

4 The d-dimensional case

We now consider the case of a d-dimensional Hamiltonian

$$H(q,p) = \frac{1}{2}p^T p + V(q)$$

where $p \in \mathbb{R}^d$ and $V : \mathbb{R}^d \mapsto \mathbb{R}$ is the potential function.

4.1 Multi-dimensional B-splines functions

Multi-dimensional B-splines approximations can be obtained rather straightforwardly from the one-dimensional case by tensor products: suppose that V takes the values $V_{n_1,\ldots,n_d}$ at the grid points

$$\begin{pmatrix} (n_1 + \frac{1}{2})\tau \\ \vdots \\ (n_d + \frac{1}{2})\tau \end{pmatrix} \tag{4.1}$$

then we define the interpolant $V^\tau(q)$ of $V(q)$ as the function

$$V^\tau(q_1,\ldots,q_d) := \sum_{(n_1,\ldots,n_d)\in\mathbb{Z}^d} V_{n_1,\ldots,n_d} \prod_{j=1}^{d} B_{n_j}(q_j) \tag{4.2}$$

where B_n is the B-splines function defined in (3.2). Proposition 3.1 can be easily generalized and is thus stated without proof:

Proposition 4.1 *Assume that V is a $\mathcal{C}^2$ function on $\mathbb{R}^d$ such that $\nabla^2 V$ is bounded on $\mathbb{R}^d$. The function V^τ defined above satisfies the estimates:*

$$\max_{q\in\mathbb{R}^d} |V(q) - V^\tau(q)| \leq C_1\tau^2 \quad \textit{and} \quad \max_{q\in\mathbb{R}^d} |\nabla V(q) - \nabla V^\tau(q)| \leq C_2\tau$$

where the constants C_1 and C_2 depend only on $\max_{q\in\mathbb{R}^d} |\nabla^2 V(q)|$.

Moreover, for a given $\tau_0 > 0$, the function $V^\tau(q)$ is uniformly $\mathcal{C}^{1,1}$ on $\mathbb{R}^d$ for $\tau \in (0, \tau_0)$.

4.2 Numerical integration of the system

For $d > 1$ and apart from specific Hamiltonians (see for instance Section 5.3), the full system with potential V^τ

$$\left\{ \begin{array}{rcl} \dot{q}(t) & = & p(t), \\ \dot{p}(t) & = & -\nabla V^\tau(q(t)), \end{array} \right. \tag{4.3}$$

can not be integrated exactly and we have to resort to the procedure described in Introduction. The vector field (4.3) is thus split into d Hamiltonian systems with hamiltonians $H^{[i,\tau]}$ defined by

$$H^{[i,\tau]}(q_i, p_i) = \frac{1}{2}p_i^2 + V^{[i,\tau]}(q_i) + \frac{1}{2}\sum_{j\neq i} \bar{p}_j^2, \tag{4.4}$$

where

$$V^{[i,\tau]}(q_i) = \sum_{n_i\in\mathbb{Z}} B_{n_i}(q_i)\bar{V}_{n_i} \text{ with } \bar{V}_{n_i} = \sum_{j\neq i}\sum_{n_j\in\mathbb{Z}} V_{n_1,\ldots,n_d}\prod_{k\neq i} B_{n_k}(\bar{q}_k),$$

which is exactly of the form (3.1): For $n_i\tau \leq q_i \leq (n_i+1)\tau$ the trajectory is obtained by solving the system

$$\left\{ \begin{array}{rcl} \dot{q}_i(t) & = & p_i(t), \\ \dot{p}_i(t) & = & \bar{\alpha}_i + \bar{\beta}_i q_i(t), \end{array} \right. \tag{4.5}$$

where

$$\begin{array}{rcl} \bar{\alpha}_i & = & \frac{1}{\tau}\left(\bar{V}_{n_i-1} - \bar{V}_{n_i} + n_i(\bar{V}_{n_i+1} - 2\bar{V}_{n_i} + \bar{V}_{n_i-1})\right), \\ \bar{\beta}_i & = & -\frac{1}{\tau^2}(\bar{V}_{n_i+1} - 2\bar{V}_{n_i} + \bar{V}_{n_i-1}), \end{array}$$

which can be done as shown in Section 3. In order to have an approximation of the solution $(q(t+h), p(t+h))$ of the full system, the equations with Hamiltonian $H^{[i,\tau]}(q_i, p_i)$ have to be solved in sequence for $i = 1, \ldots, d$. In practice, computing the exact trajectory necessitates to recompute new values of the potential $V^{[i,\tau]}$ whenever q_i crosses a frontier, since the trajectory is not on the same conic.

By combining the space approximation by B-splines functions of the potential and the time-approximation using the splitting method, we obtain the following error estimate result:

Theorem 4.2 *Let φ_t be the exact flow of the system* (1.1) *and $\varphi_{i,t}^\tau$ the exact flow of the Hamiltonian system with Hamiltonian $H^{[i,\tau]}$. The numerical flow Φ_h^τ as defined above with stepsize $h > 0$ and space discretization parameter τ is of the form $\Phi_h^\tau = \varphi_{1,h}^\tau \circ \ldots \varphi_{d,h}^\tau$ and satisfies the following estimate for all Lipschitz function g with compact support:*

$$|\langle \varphi_h - \Phi_h^\tau | g\rangle| \leq C(h\tau + h^2\|g\|_{L^1}) \tag{4.6}$$

for a constant C depending on V, and for sufficiently small h and τ.

If the systems (4.5) *are solved for $i = 1, \ldots, d$ and then for $i = d, \ldots, 1$ in reverse order, the resulting method $\Phi_{h/2}^\tau \circ \left(\Phi_{h/2}^\tau\right)^*$ is symmetric and*

$$|\langle \varphi_h - \Phi_{h/2}^\tau \circ \left(\Phi_{h/2}^\tau\right)^* |g\rangle| \leq C(h\tau + h^3\|g'\|_{L^1}). \tag{4.7}$$

Proof. Consider the componentwise vector-field splitting of $f^{[\tau]} = \nabla H^{[\tau]}$ described above and in introduction. It can be seen as the result of the splitting of $J = J_1 + \ldots + J_d$ where $(J_k)_{i,j} = \delta_{i,k}\,\delta_{j,2d-k} - \delta_{j,k}\,\delta_{i,2d-k}$. Hence, taking $n = d$ and $f_i = J_i^{-1}\nabla H^{[\tau]}$, $i = 1, \ldots, d$ in Lemma 2.6, it is clear that $\mathrm{div}(f_i) = 0$ a.e. and this proves the statements. ■

Theorem 4.3 *The numerical flow $\Phi_h^\tau = \varphi_{1,h}^\tau \circ \ldots \varphi_{d,h}^\tau$ is energy-preserving and weakly symplectic.*

Proof. This is a straightforward consequence of point (vi) of Theorem 2.2 and of the chain rule for $\varphi_{1,h}^\tau \circ \ldots \varphi_{d,h}^\tau$ which holds true since all the $\varphi_{i,h}^\tau$'s are Lipschitz functions with Lipschitz inverse. ■

5 Numerical experiments

In order to test our method with respect to the conservation of energy, volume and symmetries, we have applied it to three well-known problems of the literature.

5.1 Kepler problem

The planar equations for Kepler problem read

$$\left\{ \begin{array}{rcl} \dot{q} & = & p \in \mathbb{R}^2, \\ \dot{p} & = & -\dfrac{q}{\|q\|^{3/2}} \in \mathbb{R}^2, \end{array} \right. \tag{5.1}$$

with initial values

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}.$$

Since there is a singularity of the potential at the origin, the error of the B-splines approximation is bigger for small q's ($\|\nabla^2 V\| \approx \|q\|^{-5}$) and care should be taken that the numerical trajectory does not come too close to the origin. Big values of τ are precluded and it is clear on this example that a non-uniform grid would be much more adapted.

The accuracy of the method on a short time is shown on Figure 1 where the errors after a period are plotted for eccentricity $e = 0$ and for different values of h and τ: for sufficiently small τ and sufficiently large h, the method exhibits order 2. On the right of the figure, one can observe the typical procession of the trajectory when computed by a symplectic method. Figure 2 shows the conservation of energy over a long interval of integration and the linear growth in time of the error for a given trajectory for fixed values of τ and h.

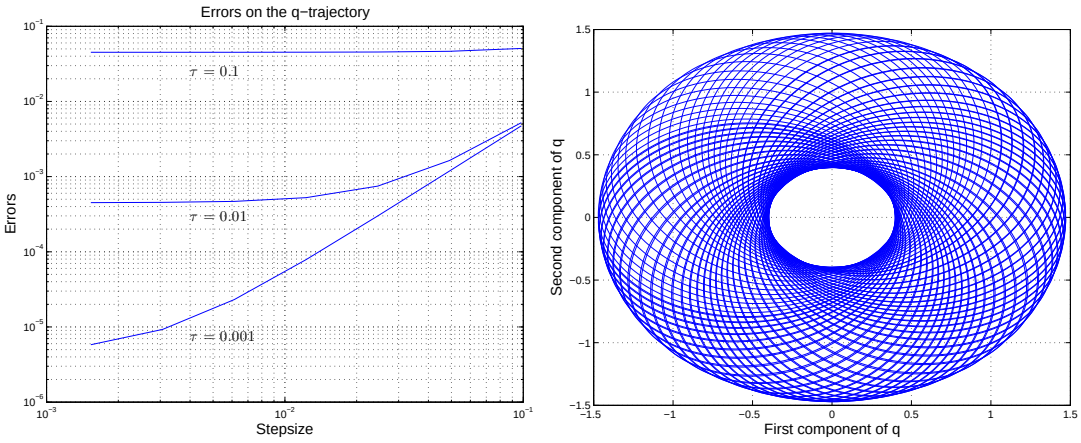

Figure 1: Errors on the trajectory and energy (left) and trajectory in the physical space (right).

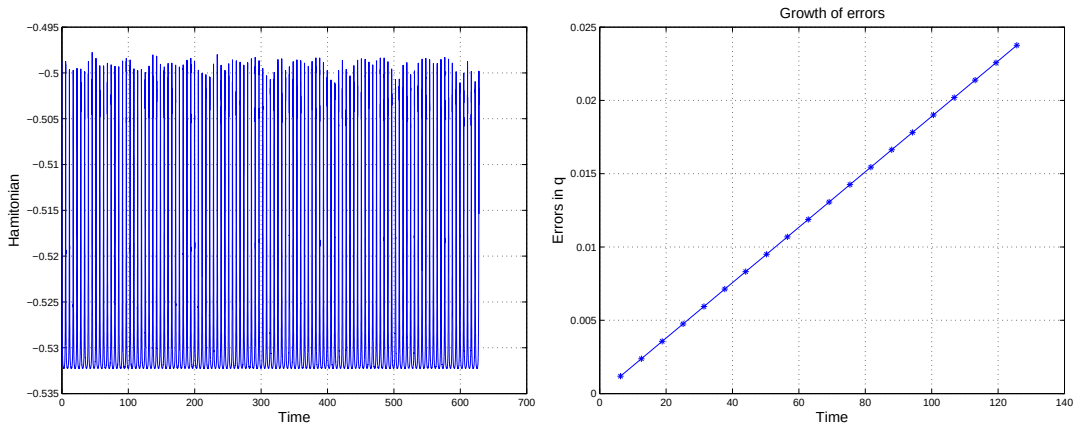

Figure 2: Energy for $e = 0.6$ with $h = \tau = 0.1$ (left) and growth with time of the error for $e = 0$, $h = 2\pi/128$, $\tau = 0.001$ (right).

5.2 Fermi-Pasta-Ulam problem

The Fermi-Pasta-Ulam problem is a highly oscillatory system with an adiabatic invariant. The Hamiltonian equations we consider are taken from [7] Sect I.4. with H given by

$$\begin{aligned} H(q,p) &= \frac{1}{2}\sum_{i=1}^{2m} p_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{2m} q_{m+i}^2 + \\ &\quad \frac{1}{4}\left((q_1 - q_{m+1})^4 + \sum_{i=1}^{m-1} (q_{i+1} - q_{m+i+1} - q_i - q_{m+i})^4 + (q - m + q_{2m})^4 \right) \end{aligned}$$

and the simulations are carried on with the initial values given therein. Figure (3) shows the computed solutions with exact solution of the subsystems and $\tau = 0.01$. For all the values

of h we have tried, no resonance occurred and the both the energy and the adiabatic invariant are conserved. Very similar figures are obtained if the one-dimensional systems are not solved

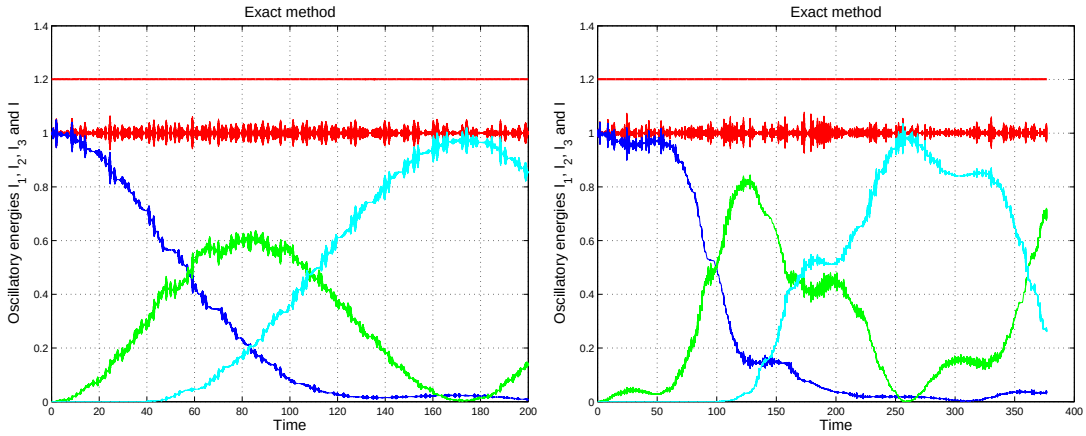

Figure 3: Preservation of energy $H - 0.8$ and adiabatic invariant I for $h = 0.01$ (left) and $h = \pi/\omega$ (right)

exactly but rather with the IMR, except that some initial values lead to a "drift" of the energy.

5.3 Sine-Gordon equation

We consider here the Sine-Gordon equation $u_{tt} = u_{xx} - \sin(u)$ with the following initial conditions

$$u(x,0) = \pi, \quad u_t(x,0) = \sin(\pi x) + \frac{1}{2}\pi^2(1-x^2),$$

taken from [6] and previously [8]. A finite differences space discretization with step $\Delta x = 2/d$, $d \in \mathbb{N}^*$, then leads to the Hamiltonian system

$$\left\{ \begin{array}{rcl} \dot{q} & = & p \\ \dot{p} & = & -\Omega^2 q - \sin(q) \end{array} \right. \tag{5.2}$$

where q is the d-dimensional vector whose j^{th}-component is an approximation of $u(x_{j-1}, t)$ at the grid point $x_{j-1} = -1 + (j-1)\Delta x$, $\sin(q)$ is the vector with components $(\sin(q_j))_{j=1,\ldots,d}$ and Ω^2 is the $d \times d$ matrix of finite differences:

$$\Omega^2 = \frac{1}{(\Delta x)^2} \begin{bmatrix} \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \ldots & 0 & \frac{1}{12} & -\frac{4}{3} \\ -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \ldots & 0 & \frac{1}{12} \\ \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \ldots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & & 0 \\ \vdots & & & & & & & \vdots \\ -\frac{4}{3} & \frac{1}{12} & 0 & \ldots & 0 & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} \end{bmatrix} \tag{5.3}$$

Its Hamiltonian is given by

$$H(q,p) = \frac{1}{2}p^T p + \frac{1}{2}q^T \Omega^2 q - \sum_{j=1}^{d} \cos(q_j) - d^2$$

and has the peculiarity to be separable in the components of q. An especially nice consequence of this is that only one quadratic approximation of $\cos$ is needed on the interval $[-\pi/2, 3\pi/2]$ and the corresponding coefficients $\hat{\beta}$ and $\hat{\alpha}$ computed once for all and then used in each box. For instance, one can take

$$\begin{aligned} \cos q_j &\approx -\frac{4}{\pi^2}q_j^2 + 1 \text{ for } -\frac{\pi}{2} \le q_j \le \frac{\pi}{2}, \\ \cos q_j &\approx \frac{4}{\pi^2}(q_j - \pi)^2 - 1 \text{ for } \frac{\pi}{2} \le q_j \le \frac{3\pi}{2}, \end{aligned}$$

i.e. $\hat{\beta}_j = -\frac{8}{\pi^2},\ \hat{\alpha}_j = 0$ on $[-\frac{\pi}{2}, \frac{\pi}{2}]$ and $\hat{\beta}_j = \frac{8}{\pi^2},\ \hat{\alpha}_j = -\frac{8}{\pi}$ on $[\frac{\pi}{2}, \frac{3\pi}{2}]$. On each box, we thus have to solve the differential equation (5.2) with Ω replaced by $\tilde{\Omega} = \Omega + \text{diag}(\hat{\beta}_1, \ldots, \hat{\beta}_d)$which admits the following exact solution.

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos(t\tilde{\Omega}) & \tilde{\Omega}^{-1}\sin(t\tilde{\Omega}) \\ -\tilde{\Omega}\sin(t\tilde{\Omega}) & \cos(t\tilde{\Omega}) \end{pmatrix} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} + \begin{pmatrix} \tilde{\Omega}^{-2}(I_d - \cos(t\tilde{\Omega}))\alpha \\ \tilde{\Omega}^{-1}\sin(t\tilde{\Omega})\alpha \end{pmatrix}.$$

Although there is no theoretical difficulties in propagating this solution, it is tricky in practice (algorithmically) to determine the exit point in a multi-dimensional cell. In this paper, we have chosen to use the method described in Section 4.2. On Figure 4, we show the numerical values of the first 32 adiabatic invariants (corresponding to the 32 smallest frequencies) computed for $h = 0.01$ (left) and $h = 0.1$ (right): note that if $\Omega = S^T D S$ with $S^T S = I$, these invariants have the form:

$$I_i = \frac{1}{2}p^T S^T \Lambda_i S p + \frac{d_{ii}}{2} q^T S^T \Lambda_i S q, \tag{5.4}$$

where $(\Lambda_i)_{j,k} = \delta_{ij}\delta_{ik}$.

6 Conclusion

The numerical method considered in this paper relies on a *grid* discretization of the potential function in the phase-space: the idea is to convert the initial problem into a sequence of more simple problems, namely Hamiltonian systems with multi-quadratic Hamiltonians, for which a splitting method introduced by R. Quispel and R. Mc Lachlan in [9] exists, that preserves both the volume and the energy.

In this work we have shown that $C^{1,1}$-approximations lead to a problem globally well-defined on the whole space which possesses an exact flow both symplectic and energy-preserving. Since the regularity of the vector-field is lower than usual (only Lipschitz), it is necessary to resort to derivatives in the sense of distributions and test-functions. These theoretical results largely explain the favorable behaviour of the method, as exhibited on test problems. However,

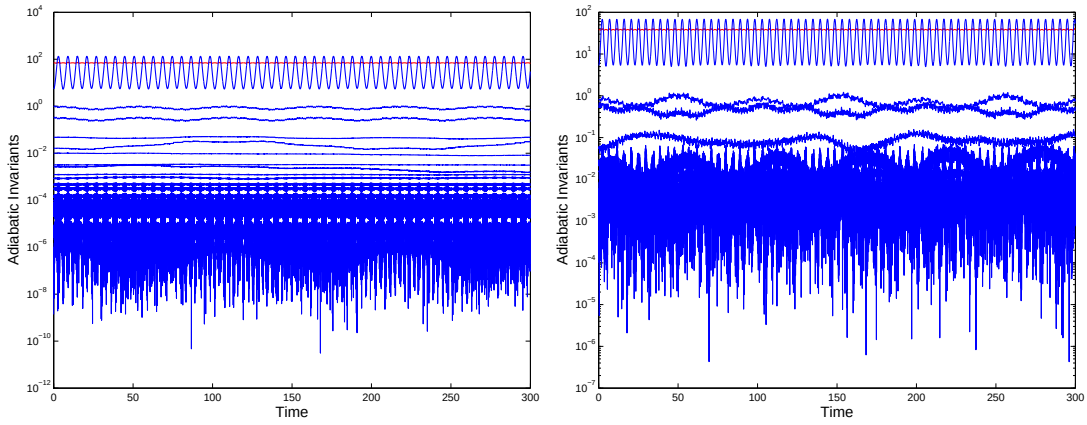

Figure 4: Preservation of energy H and adiabatic invariant I_i, $i = 1, \ldots, 32$ for $h = 0.01$ (left) and $h = 0.1$ (right)

the linear growth of the global errors observed for the Kepler equation remains unclear at this stage.

In terms of efficiency, the algorithm we developed may have a rather high computational cost compared to existing ones. This is mainly due to the approximation in space whose cost can increase dramatically with the dimension. However, it is worth mentioning two specific situations where it is of interest: the first one is encountered in image processing where the vector field is known only on a discrete grid. The second one is encountered in presence of high-oscillations of the solution: due to the use of exact trajectories the algorithm is indeed not sensitive to resonances.

Acknowledgements

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Appendix: Algorithm for the exact solution

In this section, we describe the algorithm that advances the solution by a step h while staying in the interval $]q_l, q_r[$ or by a step $0 < h_s < h$ while staying in the interval $]q_l, q_r[$ and reaching a point of the boundary at time h_s. We thus assume that $q_0 \in [q_l, q_r]$ with $q_l < q_r$ and that the trajectory enters the interval $]q_l, q_r[$.

Case of a parabole ($\beta = 0$) : The solution is of the form :

$$q(t) = q_0 + p_0 t + \alpha \frac{t^2}{2}, \tag{6.1}$$

$$p(t) = p_0 + \alpha t. \tag{6.2}$$

1. if $\alpha = 0$, then $q(t)$ is a straight line.
   (a) if $p_0 = 0$: the exit point has coordinates $q_s = q_0, \quad p_s = p_0, \quad h_s = h$.
   (b) if $p_0 > 0$: the exit point has coordinates $h_s = \min(h, (q_r - q_0)/p_0), \quad q_s = q_0 + p_0 h_s, \quad p_s = p_0$.
   (c) if $p_0 < 0$: the exit point has coordinates $h_s = \min(h, (q_l - q_0)/p_0), \quad q_s = q_0 + p_0 h_s, \quad p_s = p_0$.
2. if $\alpha > 0$ then $q = \frac{1}{2\alpha}p^2 + Q$ with $Q = q_0 - \frac{p_0^2}{2\alpha}$ is a real parabole oriented toward the positive q's.
   (a) if $p_0 < 0$ and $q_l > Q$ then let $h_s = \frac{-p_0 - \sqrt{2\alpha(q_l - Q)}}{\alpha}$.
      i. if $h_s < h$, then $q_s = q_l$ and $p_s = \alpha\, h_s + p_0$.
      ii. if $h_s > h$, then $h_s = h$, $p_s = \alpha\, h_s + p_0$ and $q_s = \frac{p_s^2}{2\alpha} + Q$.
   (b) else let $h_s = \frac{-p_0 + \sqrt{2\alpha(q_r - Q)}}{\alpha}$.
      i. if $h_s < h$, then $q_s = q_r$ and $p_s = \alpha\, h_s + p_0$.
      ii. if $h_s > h$, then $h_s = h$, $p_s = \alpha\, h_s + p_0$ and $q_s = \frac{p_s^2}{2\alpha} + Q$.
3. if $\alpha < 0$, then $q = \frac{1}{2\alpha}p^2 + Q$ with $Q = q_0 - \frac{p_0^2}{2\alpha}$, is a real parabole oriented toward the negative q's.
   (a) if $p_0 > 0$ and $q_r < Q$ then let $h_s = \frac{p_0 - \sqrt{2(-\alpha)(Q - q_r)}}{(-\alpha)}$.
      i. if $h_s < h$, then $q_s = q_r$ and $p_s = \alpha\, h_s + p_0$.
      ii. if $h_s > h$, then $h_s = h$, $p_s = \alpha\, h + p_0$ and $q_s = \frac{p_s^2}{2\alpha} + Q$.
   (b) else let $h_s = \frac{p_0 + \sqrt{2(-\alpha)(Q - q_l)}}{(-\alpha)}$.
      i. if $h_s < h$, then $q_s = q_l$ and $p_s = \alpha\, h_s + p_0$.
      ii. if $h_s > h$, then $h_s = h$, $p_s = \alpha\, h_s + p_0$ and $q_s = \frac{p_s^2}{2\alpha} + Q$.

For $\beta \neq 0$, we define the Hamiltonian as follows :

$$\begin{aligned} H(q,p) &= \frac{1}{2}p^2 - \frac{(q + \frac{\alpha}{\beta})^2}{2\beta^{-1}} \\ &= \frac{1}{2}p^2 - \frac{\psi^2}{2\beta^{-1}} := \tilde{H}(\psi, p), \end{aligned}$$

where $\psi = q + \frac{\alpha}{\beta}$. Eventually, we denote $a = \sqrt{2|\beta^{-1}||\tilde{H}_0|}$, $b = \sqrt{2|\tilde{H}_0|}$ and $\omega = \sqrt{|\beta|}$.

Case of an ellipse ($\beta < 0$ and hence $\tilde{H}_0 \geq 0$) :

1. if $\tilde{H}_0 = 0$: singularity of the vector field!

2. the trajectory is a piece of the ellipse $\mathcal{E}$ with cartesian equation $\frac{\psi^2}{a^2} + \frac{p^2}{b^2} = 1$ and parametric equations $\psi(t) = a\cos(\varphi_0 - \omega t), p(t) = b\sin(\varphi_0 - \omega t)$.

   (a) $p_0 > 0$ or ($p_0 = 0$ and $\psi_0 < 0$) : $\varphi_0 = \arccos(\psi_0/a)$. We look whether $\mathcal{E}$ crosses $\psi = \psi_r$ and then $\psi = \psi_l$.

      i. if $\psi_r < a$, then the exit point has coordinates

$$\psi_s = \psi_r, \quad p_s = +b\sqrt{1 - \frac{\psi_r^2}{a^2}}, \quad h_s = \omega^{-1}(\varphi_0 - \arccos(\psi_s/a)). \quad (6.3)$$

      ii. if $\psi_r \geq a$:

         A. if $\psi_l > -a$, then the exit point has coordinates

$$\psi_s = \psi_l, \quad p_s = -b\sqrt{1 - \frac{\psi_l^2}{a^2}}, \quad h_s = \omega^{-1}(\varphi_0 + \arccos(\psi_s/a)). \quad (6.4)$$

         B. if $\psi_l \leq -a$: $\mathcal{E}$ is fully contained in the ψ-band. $h_s = h$, $\psi(h_s) = a\cos(\varphi_0 - \omega h_s), p(h_s) = b\sin(\varphi_0 - \omega h_s)$.

   (b) $p_0 < 0$ or ($p_0 = 0$ and $\psi_0 > 0$) : $\varphi_0 = -\arccos(\psi_0/a)$. We look whether $\mathcal{E}$ crosses $\psi = \psi_l$ and then $\psi = \psi_t$.

      i. if $\psi_l > -a$, then the exit point has coordinates

$$\psi_s = \psi_l, \quad p_s = -b\sqrt{1 - \frac{\psi_l^2}{a^2}}, \quad h_s = \omega^{-1}(\varphi_0 + \arccos(\psi_s/a)). \quad (6.5)$$

      ii. if $\psi_l \leq -a$,

         A. if $\psi_r < a$, then the exit point has coordinates

$$\psi_s = \psi_r, \quad p_s = +b\sqrt{1 - \frac{\psi_r^2}{a^2}}, \quad h_s = \omega^{-1}(\varphi_0 + 2\pi - \arccos(\psi_s/a)). \quad (6.6)$$

         B. if $\psi_r \geq a$: $\mathcal{E}$ is fully contained in the ψ-band. $h_s = h$, $\psi(h_s) = a\cos(\varphi_0 - \omega h_s), p(h_s) = b\sin(\varphi_0 - \omega h_s)$.

Case of an hyperbole ($\beta > 0$:)

1. if $\tilde{H}_0 = 0$: the trajectory is a straight line with equation $\varepsilon(p_0)p = \varepsilon(\psi_0)\omega\psi$.

2. if $\tilde{H}_0 < 0$: the trajectory is a piece of the hyperbole

$$\frac{\psi^2}{a^2} - \frac{p^2}{b^2} = 1, \quad \begin{array}{rcl} \psi & = & \varepsilon(\psi_0)\, a\, \cosh(\varepsilon(\psi_0)t + t_0) \\ p & = & b\sinh(\varepsilon(\psi_0)t + t_0) \end{array}, \quad t_0 \;=\; \text{Argsh}\left(\frac{p_0}{b}\right).$$

   (a) if $\psi_0 > 0$:

      i. if $p_0 < 0$ and $\psi_l > a$ then $\psi_s = \psi_l$ and $p_s = -\frac{b}{a}\sqrt{\psi_s^2 - a^2}$

ii. else $\psi_s = \psi_r$ and $p_s = \frac{b}{a}\sqrt{\psi_s^2 - a^2}$

(b) if $\psi_0 < 0$:

i. if $p_0 > 0$ and $\psi_r < -a$ then $\psi_s = \psi_r$ and $p_s = \frac{b}{a}\sqrt{\psi_s^2 - a^2}$

ii. else $\psi_s = \psi_l$ and $p_s = -\frac{b}{a}\sqrt{\psi_s^2 - a^2}$

Then $h_s = \varepsilon(\psi_0)\left(\text{Argsh}(p_s/b) - \text{Argsh}(p_0/b)\right)$. If $h_s > h$ then $h_s = h$ and

$$\begin{aligned} \psi_s &= \varepsilon(\psi_0)\frac{a}{b}\left(\sqrt{p_0^2 + b^2}\cosh(h) + \sinh\left(\varepsilon(\psi_0)\, h\right) p_0\right), \\ p_s &= \sqrt{p_0^2 + b^2}\sinh(\varepsilon(\psi_0)h) + \cosh(h)p_0. \end{aligned}$$

3. if $\tilde{H}_0 > 0$: the trajectory is a piece of the hyperbole

$$\frac{p^2}{b^2} - \frac{\psi^2}{a^2} = 1, \qquad \begin{aligned} p &= \varepsilon(p_0)\, b\, \cosh(\varepsilon(p_0)t + t_0), \\ \psi &= a\sinh(\varepsilon(p_0)t + t_0), \end{aligned} \qquad t_0 = \text{Argsh}\left(\frac{\psi_0}{a}\right).$$

Let

$$\psi_s = \frac{1 + \varepsilon(p_0)}{2}\psi_r + \frac{1 - \varepsilon(p_0)}{2}\psi_l \text{ and } h_s = \varepsilon(p_0)\left(\text{Argsh}(\psi_s/a) - \text{Argsh}(\psi_0/a)\right).$$

If $h_s > h$, then $h_s = h$ and

$$\psi_s = \sinh\left(\varepsilon(p_0)\, h\right)\sqrt{{\psi_0}^2 + a^2} + \cosh\left(h\right)\psi_0.$$

Eventually,

$$p_s = \varepsilon(p_0)\frac{b}{a}\sqrt{\psi_s^2 + a^2}.$$

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