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Abstract

Symplectic methods, like the Verlet method, are a standard tool for the long term integration of Hamiltonian systems as they arise, for example, in molecular dynamics. One of the reasons for the popularity of symplectic methods is the conservation of energy over very long periods of time up to small fluctuations that scale with the order of the method. In this paper, we discuss a qualitative feature of Hamiltonian systems with separated time scales that is also preserved under symplectic discretization. Specifically, highly oscillatory degrees of freedom often lead to almost preserved quantities (adiabatic invariants). Using recent results from backward error analysis and normal form theory, we show that a symplectic method, like the Verlet method, preserves those adiabatic invariants. We also discuss step-size restrictions necessary to maintain adiabatic invariants in practical computations.

1 Introduction

It is well-known (see [12], for example) that symplectic discretization schemes possess particularly attractive properties when applied over long time[1] to Hamiltonian systems

$$\begin{aligned} \frac{d}{dt}q &= M^{-1}p\,, \\ \frac{d}{dt}p &= -\nabla_q V(q)\,, \end{aligned}$$

$q,p \in R^n$, $V : R^n \to R$ the potential energy function, and M the positive definite mass matrix. In fact, it can be shown that a symplectic method such as the Verlet method [15]

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{\Delta t}{2}\nabla_q V(q_n)\,, \\ q_{n+1} &= q_n + \Delta t M^{-1} p_{n+1/2}\,, \\ p_{n+1} &= p_{n+1/2} - \frac{\Delta t}{2}\nabla_q V(q_{n+1})\,, \end{aligned}$$

[1] One must consider $N\,\Delta t \gg 1$, where Δt is the discretization step-size and N is the number of discretization steps.

can be considered as the "almost" exact solution to a modified Hamiltonian system [5, 7, 10]. The remarkable consequence of this backward error approach is the conservation of energy by a symplectic integrator [5, 7, 10]. To be more precise: The symplectic method will conserve a modified Hamiltonian $\tilde{H}$ which, due to the discretization error of the method, is $\mathcal{O}(\Delta t^p)$, $p \geq 1$ the order of the method, away from the given Hamiltonian

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

Thus, if we plot the energy function H along the numerically computed trajectories, we will observe $\mathcal{O}(\Delta t^p)$ fluctuations about the initial value of H but no secular drift. Note that the energy function $\tilde{H}$ is known to exists by backward error analysis but, except for simple cases, is difficult to compute explicitly.

Conservation of energy by a symplectic method cannot explain the success of such methods in long term simulations such as molecular dynamics. The reason is that any numerically method can be forced to conserve energy by a simple projection step onto the hypersurface of constant energy. In this paper, we like to bring forward another reason for the superiority of symplectic methods in long term simulations. In particular, we will look at Hamiltonian systems with two well separated time scales with the fast motion being highly oscillatory. Theoretical results predict that (at least in the case of a single fast degree of motion) the system will possess an adiabatic invariant [1], i.e., there is a quantity that is practically conserved along trajectories. Note that an adiabatic invariant is not a first integral although both lead to conserved quantities. While a first integral is related to symmetries, adiabatic invariants are caused by the existence of different time scales in the solution behavior. We will show that a symplectic method such as Verlet will conserve the adiabatic invariant provided the step-size is chosen small enough. This result seems important. Adiabatic invariants are often hidden, i.e., are not explicitly given like the energy function H. Thus a non-symplectic energy conserving scheme might lead to qualitatively wrong results because of the non-conservation of the "hidden" adiabatic invariant(s).

The paper is organized as follows: In Section 2, the model problem is introduced and first numerical results are presented. In Section 3, the numerical findings are explained theoretically. Our analysis is based on normal form theory [1] and backward error analysis [12]. More advanced topics concerning step-size restrictions are discussed in the final section. For a discussion on related issues in the context of implicit symplectic methods and very large step-size integration (w.r.t. the fast motion) see Ascher & Reich [2].

2 The Model Problem

Let us consider a Hamiltonian system with a single highly oscillatory degree of freedom, i.e., a system of type

$$\frac{d}{dt}q \;=\; M^{-1}p\,, \tag{1}$$

$$\frac{d}{dt}p \;=\; -\nabla_q V(q) - \epsilon^{-2} g(q) \nabla_q g(q) \tag{2}$$

with Hamiltonian

$$H(q,p;\epsilon) \;=\; \frac{p^T M^{-1} p}{2} + V(q) + \frac{\epsilon^{-2}}{2} g(q)^2 \,. \qquad (3)$$

Here $0 < \epsilon < \epsilon_0$ is a small parameter and $g : R^n \to R$ a smooth function such that the Jacobian $g'(q)$ satisfies $|g'(q)| > d$ for $q \in g^{-1}(0)$, $d > 0$ an appropriate constant. Without loss of generality, we set $M = I$ and restrict ourselves to systems with two degrees of freedom, i.e., $q, p \in R^2$.

The behavior of our model system becomes more apparent when going to (local) coordinates $x := g(q)$ and $y := b(q)$. Here $b : R^2 \to R$ is an appropriate function such that $g'(q)b'(q)^T = 0$ for all q in the domain of the coordinate transformation. The corresponding conjugate momenta p_x and p_y are implicitly defined by the relation

$$p \;=\; p_x \nabla_q g(q) + p_y \nabla_q b(q) \,.$$

Thus we end up with the transformed Hamiltonian system

$$\begin{aligned}
\frac{d}{dt} x &= m_x(x,y) p_x \,, \\
\frac{d}{dt} p_x &= -\epsilon^{-2} x - \nabla_x V(x,y) - \frac{1}{2} \nabla_x \left[m_x(x,y) p_x^2 + m_y(x,y) p_y^2 \right] \,, \\
\frac{d}{dt} y &= m_y(x,y) p_y \,, \\
\frac{d}{dt} p_y &= -\nabla_y V(x,y) - \frac{1}{2} \nabla_y \left[m_x(x,y) p_x^2 + m_y(x,y) p_y^2 \right]
\end{aligned}$$

with $m_x(x,y) := g'(q)g'(q)^T$ and $m_y(x,y) := b'(q)b'(q)^T$.

The initial conditions are chosen such that the corresponding total energy $H(\epsilon)$ remains bounded as $\epsilon \to 0$. Thus, by conservation of the total energy $H(\epsilon) = \mathcal{O}(1)$ we know that $x(t) = \mathcal{O}(\epsilon)$ and we rescale x by ϵ, i.e., we replace $\epsilon^{-1} x$ by $\tilde{x}$. This yields the system

$$\begin{aligned}
\frac{d}{dt} \tilde{x} &= \epsilon^{-1} m_x(\epsilon\tilde{x},y) p_x \,, \\
\frac{d}{dt} p_x &= -\epsilon^{-1} \tilde{x} - \nabla_x V(\epsilon\tilde{x},y) - \frac{1}{2} \nabla_x \left[m_x(\epsilon\tilde{x},y) p_x^2 + m_y(\epsilon\tilde{x},y) p_y^2 \right] \,, \\
\frac{d}{dt} y &= m_y(\epsilon\tilde{x},y) p_y \,, \\
\frac{d}{dt} p_y &= -\nabla_y V(\epsilon\tilde{x},y) - \frac{1}{2} \nabla_y \left[m_x(\epsilon\tilde{x},y) p_x^2 + m_y(\epsilon\tilde{x},y) p_y^2 \right]
\end{aligned}$$

which is still Hamiltonian but with a modified Lie-Poisson bracket (see [10] for details). The motion in $(\tilde{x}, p_x)$ is highly oscillatory. To make this more transparent, we introduce action-angle variables[2] $(J, \phi) \in R \times S$ via

$$\begin{aligned}
\tilde{x} &= \sqrt{2\omega(y) J} \cos\phi \,, \\
p_x &= \sqrt{\frac{2J}{\omega(y)}} \sin\phi \,,
\end{aligned}$$

[2]Because ω depends on y, the symplectic transformation to action-angle variables is non-trivial. In fact, the transformation also involves a small $\mathcal{O}(\epsilon)$ change in the momentum p_y which, for notational convenience, we skip here. See [10] for details.

and

$$J := \frac{1}{2\omega(y)} \left[\omega(y)^2 p_x^2 + \tilde{x}^2\right] , \tag{4}$$

$\omega(y) = \sqrt{m_x(0,y)}$, which finally gives us a system of type (see [10] again for details)

$$\begin{aligned}
\frac{d}{dt}\phi &= \epsilon^{-1}\omega(y) + \nabla_J f(\phi, J, y, p_y; \epsilon) , \\
\frac{d}{dt}J &= -\nabla_\phi f(\phi, J, y, p_y; \epsilon) , \\
\frac{d}{dt}y &= \nabla_{p_y} h(y, p_y) + \epsilon \nabla_{p_y} f(\phi, J, y, p_y; \epsilon) , \\
\frac{d}{dt}p_y &= -\nabla_y h(y, p_y) - \epsilon \nabla_y f(\phi, J, y, p_y; \epsilon) - \nabla_y \omega(y) J .
\end{aligned}$$

Here f and h are well-defined functions. The corresponding Hamiltonian is

$$\mathcal{H}(\phi, J, y, p_y; \epsilon) = \omega(y)J + h(y, p_y) + \epsilon f(\phi, J, y, p_y; \epsilon) \tag{5}$$

and the equations of motion are generated via (the non-canonical Lie-Poisson structure)

$$\begin{aligned}
\frac{d}{dt}\phi &= \epsilon^{-1}\nabla_J \mathcal{H}(\phi, J, y, p_y; \epsilon) , \\
\frac{d}{dt}J &= -\epsilon^{-1}\nabla_\phi \mathcal{H}(\phi, J, y, p_y; \epsilon) , \\
\frac{d}{dt}y &= \nabla_{p_y} \mathcal{H}(\phi, J, y, p_y; \epsilon) , \\
\frac{d}{dt}p_y &= -\nabla_y \mathcal{H}(\phi, J, u, p_y; \epsilon) .
\end{aligned}$$

This certainly looks complicated. However, it allows us to apply normal form theory which implies the adiabatic invariance of the action J. This will be discussed in more detail in Section 3.

Let us give a brief history of our model problem. First theoretical results were published by Rubin & Ungar [11] and Takens [14]. These authors gave results on the limiting behavior as $\epsilon \to 0$. More recently, Borneman & Schütte [6] gave a different derivation for the limiting behavior using homogenization techniques. Normal form theory has been used for the special case of $\omega = const.$ by Benettin, Galgani & Gorgilli [4] which allows one to derive estimates on the variations in the adiabatic invariant J for finite ϵ. A discussion of the general case (non-constant ω) in terms of normal form theory can be found in [10].

Example. Let us define the function g in (1)-(2) by

$$g(q) = \sqrt{a q_1^2 + b q_2^2} - 1 .$$

For $a = b = 1$, we obtain $g(q) = r(q) - 1$ which is the stiff spring pendulum [2]. As the potential energy function V we chose $V(q) = q_1$. Thus the equations of motion are

$$
\begin{aligned}
\frac{d}{dt}q_1 &= p_1\,, \\
\frac{d}{dt}q_2 &= p_2\,, \\
\frac{d}{dt}p_1 &= -a\frac{\sqrt{aq_1^2+bq_2^2}-1}{\sqrt{aq_1^2+bq_2^2}}q_1 - 1\,, \\
\frac{d}{dt}p_2 &= -b\frac{\sqrt{aq_1^2+bq_2^2}-1}{\sqrt{aq_1^2+bq_2^2}}q_2\,.
\end{aligned}
$$

Next we have to find an expression for the adiabatic invariant J. Using general expression (4), this requires the energy H_x in the fast x-degree of freedom:

$$
\begin{aligned}
H_x &= \omega(y)^2\frac{p_x^2}{2} + \frac{\epsilon^{-2}}{2}x^2\,, \\
&= \frac{p^T g'(q)^T[g(q)g'(q)^T]^{-1}g'(q)p}{2} + \frac{\epsilon^{-2}}{2}g(q)^2\,.
\end{aligned}
$$

Here we have used that $p_x = [g'(q)g'(q)^T]^{-1}g'(q)p$. The frequency ω is defined by

$$
\omega = \sqrt{\frac{a^2q_1^2+b^2q_2^2}{aq_1^2+bq_2^2}}\,.
$$

Thus $J = H_x/\omega$. Numerical experiments using the Verlet method were conducted for $a = 2$ and $b = 1$, $\epsilon = 0.01, 0.02, 0.04$, and step-sizes $\Delta t \le \epsilon$. The initial conditions were $(q,p) = (-\sqrt{0.5}, 0, 1, 1)$. The numerical results can be found in Table 1 with

$$
\Delta J := \max_{t_n\in[0,100]} |J(0) - J(t_n)| \qquad \text{and} \qquad \Delta H := \max_{t_n\in[0,100]} |H(0) - H(t_n)|\,.
$$

One can clearly see the quadratic convergence of the energy error as $\Delta t/\epsilon \to 0$. It is also obvious that, for $\Delta t/\epsilon$ small enough, the error in the adiabatic invariant depends linearly on ϵ. For large $\Delta t/\epsilon$ the error in the adiabatic invariant is dominated by the discretization error. Note that, for $\Delta t/\epsilon \approx 1$, the high-frequency oscillations in the (x,p_x)-degree of freedom are not correctly reproduced. Still neither the energy nor the adiabatic invariant show any secular drift. We will come back to this phenomenon in Section 4. $\square$

3 Theoretical Results for Small Step-Sizes

In this section we review some basic results of backward error analysis and normal form theory from the prospective of our model problem and its Verlet discretization. For that reason, let us first introduce some notations. We write the Verlet method as

$$
z_{n+1} = \Psi_{\Delta t}(z_n)\,, \qquad z = (q^T, p^T)^T \in R^4\,.
$$

Δt	ϵ	$\Delta t/\epsilon$	ΔJ	ΔH
0.5e-3	0.1e-1	0.5e-1	0.10e-1	0.63e-3
0.1e-2	0.1e-1	0.1	0.11e-1	0.25e-2
0.2e-2	0.1e-1	0.2	0.16e-1	0.10e-1
0.4e-2	0.1e-1	0.4	0.40e-1	0.43e-1
0.8e-2	0.1e-1	0.8	0.17	0.23
0.1e-1	0.1e-1	1.0	0.36	0.50
0.5e-3	0.2e-1	0.25e-1	0.20e-1	0.16e-3
0.1e-2	0.2e-1	0.5e-1	0.20e-1	0.63e-3
0.2e-2	0.2e-1	0.1	0.21e-1	0.25e-2
0.4e-2	0.2e-1	0.2	0.26e-1	0.10e-1
0.8e-2	0.2e-1	0.4	0.48e-1	0.43e-1
0.1e-1	0.2e-1	0.5	0.69e-1	0.70e-1
0.2e-1	0.2e-1	1.0	0.38	0.50
0.5e-3	0.4e-1	0.12e-1	0.40e-1	0.39e-4
0.1e-2	0.4e-1	0.25e-1	0.40e-1	0.16e-3
0.2e-2	0.4e-1	0.5e-1	0.40e-1	0.63e-3
0.4e-2	0.4e-1	0.1	0.41e-1	0.25e-2
0.8e-2	0.4e-1	0.2	0.46e-1	0.10e-1
0.1e-1	0.4e-1	0.25	0.50e-1	0.15e-1
0.2e-1	0.4e-1	0.5	0.88e-1	0.70e-1
0.4e-1	0.4e-1	1.0	0.40	0.50

Table 1: Preservation of the adiabatic invariant J and total energy H under the Verlet discretization.

The equations of motion are given more compactly by

$$\frac{d}{dt}z \;=\; \{\mathrm{id}, H(\epsilon)\}(z)$$

$\{.,.\}$ the canonical Lie-Poisson bracket, $H(\epsilon)$ the Hamiltonian (3) and $\mathrm{id} : R^4 \to R^4$ the identity map. The time-t-flow map is denoted by $\Phi_{t,H}$. We also assume that the Hamiltonian $H(\epsilon)$ is real-analytic on an appropriate (compact) subset $\mathcal{K}$ of phase space and that the real analytic vector field $Z_H := \{\mathrm{id}, H(\epsilon)\}$ is bounded on a complex neighborhood[3] $\mathcal{B}_R\mathcal{K}$ of $\mathcal{K}$. For our model problem, this bound will, typically, be of the form

$$||\,\{\mathrm{id}, H(\epsilon)\}(z)\,|| \;\leq\; \epsilon^{-1} M\,, \qquad z \in \mathcal{B}_R\mathcal{K}\,,$$

$M > 0$ an appropriate constant, for all $\epsilon \leq \epsilon_0$.

For a symplectic method like Verlet, backward error analysis is concerned with finding a family of modified Hamiltonian functions $\tilde{H}(\epsilon, \Delta t)$ such that the time-Δt-flow map $\Phi_{\Delta t,\tilde{H}}$ of the corresponding Hamiltonian vector field $Z_{\tilde{H}}$ is "equivalent" to the discretization map $\Psi_{\Delta t}$. As first shown by Neishtadt[4] [9], the difference between $\Phi_{\Delta t,\tilde{H}}$ and $\Psi_{\Delta t}$ can be made exponentially small in Δt. For our model problem and the Verlet discretization, we obtain in particular

$$||\,\Psi_{\Delta t}(z) - \Phi_{\Delta t,\tilde{H}}(z)\,|| \;\leq\; c_1\,\alpha\, e^{-c_2/\alpha}\,, \qquad \alpha := \epsilon^{-1}\Delta t\,,$$

for all $\alpha \leq \alpha_0$. Here $c_1, c_2 > 0$ are appropriate constants proportional to M/R and $\alpha_0 > 0$ some constant with $\alpha_0 \leq c_2$ [10]. Note that, for the Verlet method, the Taylor expansion of the modified Hamiltonian $\tilde{H}(\epsilon, \Delta t)$ w.r.t. Δt is given by the Baker-Campbell-Hausdorff formula [12]. Thus $\tilde{H}(\epsilon, \Delta t)$ is known to exist globally on $\mathcal{K}$. Since the Verlet method is second order, the modified Hamiltonian $\tilde{H}$ satisfies

$$\tilde{H}(\epsilon, \Delta t) \;=\; H(\epsilon) + \alpha^2 \Delta H(\epsilon, \Delta t) \tag{6}$$

with $H(\epsilon)$ given by (3) and

$$|\,\Delta H(z; \epsilon, \Delta t)\,| \;\leq\; c_3\,, \qquad z \in \mathcal{B}_{R/2}\mathcal{K}\,,$$

$c_3 > 0$ a constant proportional to M/R.

In the sequel, we assume that the numerically computed solutions stay on the (compact) subset $\mathcal{K}$ throughout the whole numerical integration. This implies conservation of the Hamiltonian $H(\epsilon)$ up to terms of order $\mathcal{O}(\alpha^2)$, $\alpha = \Delta t/\epsilon$, over exponentially long integration intervals provided α is sufficiently small. For example, $\Delta t = \mathcal{O}(\epsilon^2)$ which, however, leads to extremely small time steps. We will come back to this issue in Section 4. The α-dependence of fluctuations in the numerically computed $H(q_n, p_n; \epsilon)$ is indeed confirmed by our results in Table 1.

Let us now investigate the conservation of the adiabatic invariant J under the Verlet discretization. For that reason, we transform the modified Hamiltonian (6) to (ϕ, J, y, p_y) coordinates and denote the result by $\tilde{\mathcal{H}}(\epsilon, \Delta t)$, i.e.

$$\tilde{\mathcal{H}}(\epsilon, \Delta t) \;=\; \mathcal{H}(\epsilon) + \alpha^2 \Delta\mathcal{H}(\epsilon, \Delta t) \tag{7}$$

[3] $\mathcal{B}_R\mathcal{K}$ is the union of complex balls of radius R around each $z \in \mathcal{K}$

[4] Different proofs for the same result were given by Benettin & Giorgilli [5], Hairer & Lubich [7], and Reich [10]

with

$$|\,\Delta\mathcal{H}(\phi,J,y,p_y;\epsilon,\Delta t)\,| \;\;\le\;\; \hat{c}_3\,, \qquad (\phi,J,y,p_y)\;\in\;\mathcal{B}_{\hat{R}/2}\hat{\mathcal{K}}\,,$$

for $\epsilon \le \epsilon_0$ and Δt sufficiently small. Here superscript "hat" denotes the corresponding transformed quantities. Using (5), we rewrite (7) as

$$\begin{aligned}
\tilde{\mathcal{H}}(\epsilon,\Delta t) &= \omega(y)J + h(y,p_y) + \epsilon f(\phi,J,y,p_y;\epsilon) + \alpha^2\Delta\mathcal{H}(\phi,J,y,p_y;\epsilon,\Delta t)\,,\\
&= \omega(y)J + h(y,p_y) + \delta\, w(\phi,J,y,p_y;\epsilon,\Delta t)\,,
\end{aligned}$$

with

$$\delta\, w(\phi,J,y,p_y;\epsilon,\Delta t) \;\;:=\;\; \epsilon f(\phi,J,y,p_y;\epsilon) + \alpha^2\Delta\mathcal{H}(\phi,J,y,p_y;\epsilon,\Delta t)$$

and $\delta := \epsilon + \hat{c}_3\alpha^2$, and apply normal form theory with δ as the small parameter[5]. In particular, let us assume that $|\omega(y)| \ge 1$, $|h(y,p_y)| \le d$, $|w(\phi,J,y,p_y;\epsilon,\Delta t)| \le d$, and $|\omega'(y)| \le 1$ for all $(\phi,J,y,p_y) \in \mathcal{B}_{\hat{R}/2}\hat{\mathcal{K}}$, $\epsilon \le \epsilon_0$, and $\alpha \le \alpha_0$, $d > 0$ some moderate constant. Then there exists a symplectic change of coordinates (w.r.t. the non-canonical Lie-Poisson structure) that transforms the Hamiltonian $\tilde{\mathcal{H}}(\epsilon,\Delta t)$ to

$$\bar{\mathcal{H}}(\epsilon,\Delta t) \;\;=\;\; \omega(\bar{y})\bar{J} + h(\bar{y},\bar{p}_y) + \delta\bar{w}(\bar{J},\bar{y},\bar{p}_y;\epsilon,\Delta t) + \mathcal{O}(e^{-c_4/\delta})$$

with

$$\delta \;\;=\;\; \epsilon + \hat{c}_3\alpha^2\,, \qquad \alpha \;=\; \Delta t/\epsilon$$

as before and $c_4 > 0$ an appropriate constant. Thus, up to an exponentially small truncation error in δ, the action $\bar{J}$ is a first integral of the transformed system (since $\bar{w}$ does not depend on $\bar{\phi}$). According to normal form theory [9, 10], the change of coordinates is δ-close to the identity and the original action J is preserved up to terms of $\mathcal{O}(\delta)$ over an exponentially long period of time. Depending on whether $\epsilon \gg \alpha$ or $\epsilon \ll \alpha$, we will see an ϵ-dependence or an α-dependence in the numerically computed action $J(t)$. This is indeed confirmed by looking at Table 1.

The results, outlined so far, are an example of a Hamiltonian system where the Hamiltonian perturbation introduced by the numerical integration does not alter the solution behavior in an essential way (at least w.r.t. the adiabatic invariant J) [5]. The conservation of adiabatic invariants under symplectic discretization has also been confirmed numerically for other test problems. See, for example, the results by Baldan & Benettin [3] on the "freezing" of fast rotations.

The life-span of the backward error analysis depends on the smallness of α while the life-span of the normal form truncation depends on the smallness of δ. To have $\alpha \sim \delta \sim \epsilon$, one has to apply a step-size $\Delta t = \mathcal{O}(\epsilon^2)$ which, as pointed out before, seems very inefficient. In particular, the Verlet method yields a stable discretization of a harmonic oscillator with frequency ϵ^{-1} provided $\Delta t \le 2\epsilon$ which corresponds to $\alpha \le 2$ [13]. Clearly, backward error analysis as presented here cannot be applied in this case. This becomes also obvious from the numerical results presented in Table 1 (note the large fluctuations in energy and the adiabatic invariant for $\alpha = 1$). Still we obtained stable numerically results. An effect we like to explain in the following section.

[5]The basic result is again due to Neishtadt [9]. However, his proof requires modifications since we work with a non-canonical Lie-Poisson structure [10]. A different proof has also been given by Benettin, Galgani & Giorgilli [4] for the case of constant ω.

4 Larger Step-Sizes and Backward Errors

For $\alpha = \Delta t/\epsilon$ close to one, the motion in the highly oscillatory (x, p_x) degree of freedom is not resolved accurately. However, the motion in (x, p_x) is basically harmonic (with slowly varying frequency):

$$\begin{aligned} \frac{d}{dt}x &= \omega^2 p_x \,, \\ \frac{d}{dt}p_x &= -\epsilon^{-2} x \,. \end{aligned}$$

Here $\omega = \omega(y)$ is kept constant for the moment. The Verlet discretization applied to this harmonic oscillator yields the (linear) one-step map

$$\begin{pmatrix} x_{n+1} \\ p_{x,n+1} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\Delta t \omega^2}{2\epsilon^2} & \Delta t \omega^2 \\ -\frac{\Delta t}{\epsilon^2}\left(1 + \frac{\Delta t^2 \omega^2}{4\epsilon^2}\right) & 1 - \frac{\Delta t \omega^2}{2\epsilon^2} \end{pmatrix} \begin{pmatrix} x_n \\ p_{x,n} \end{pmatrix}$$

which, since the Verlet method is symplectic, can be considered as the exact (!) time-Δt-flow map of the modified harmonic oscillator

$$\begin{aligned} \frac{d}{dt}x &= c\omega_{eff}^2 p_x \,, \\ \frac{d}{dt}p_x &= -c^{-1}\epsilon^{-2} x \end{aligned}$$

with

$$\omega_{eff}(\alpha) \;:=\; \frac{2\epsilon}{\Delta t}\arcsin\left(\frac{\omega \Delta t}{2\epsilon}\right)$$

and

$$c \;:=\; \frac{\omega}{\omega_{eff}}\left(1 - \frac{\Delta t^2 \omega^2}{4\epsilon^2}\right)^{-1/2} .$$

The corresponding Hamiltonian is

$$K_x(x, p_x, y; \alpha, \epsilon) \;:=\; \frac{c}{2}\left(\omega_{eff}(y;\alpha)^2 p_x^2 + c^{-2}\epsilon^{-2} x^2\right)$$

which is exactly conserved by the linear Verlet map[6]. This suggests to replace the harmonic part H_x of the given model problem by the modified Hamiltonian K_x. This should take care of the largest contributions to the local error for $\alpha \sim 1$. Thus we define the following modified Hamiltonian

$$K(q, p; \alpha, \epsilon) \;:=\; K_x(x, p_x, y; \alpha, \epsilon) + \frac{p^T b'(q)^T [b'(q) b'(q)^T]^{-1} b'(q) p}{2} + V(q)$$

with $\omega = \sqrt{g'(q) g'(q)^T}$, $x = g(q)$, and p_x defined by

$$p_x \;:=\; [g'(q) g'(q)^T]^{-1} g'(q) p \,.$$

[6]The concept of postprocessing as used, for example, by Skeel, Zhang & Schlick in [13] leads to the same result. However, the modified Hamiltonian approach used here fits better to the concept of backward error analysis.

Δt	ϵ	$\Delta t/\epsilon$	ΔJ_{mod}	ΔK	$\Delta\omega$
0.2e-2	0.1e-1	0.2	0.10e-1	0.81e-4	0.48e-2
0.4e-2	0.1e-1	0.4	0.10e-1	0.35e-3	0.20e-1
0.8e-2	0.1e-1	0.8	0.10e-1	0.18e-2	0.90e-1
0.1e-1	0.1e-1	1.0	0.12e-1	0.37e-2	0.16
0.4e-2	0.2e-1	0.2	0.20e-1	0.16e-3	0.48e-2
0.8e-2	0.2e-1	0.4	0.20e-1	0.70e-3	0.20e-1
0.1e-1	0.2e-1	0.5	0.20e-1	0.11e-2	0.32e-1
0.2e-1	0.2e-1	1.0	0.23e-1	0.75e-2	0.16
0.1e-1	0.4e-1	0.25	0.40e-1	0.52e-3	0.75e-2
0.2e-1	0.4e-1	0.5	0.40e-1	0.23e-2	0.32e-1
0.4e-1	0.4e-1	1.0	0.47e-1	0.15e-1	0.16
0.5e-1	0.4e-1	1.25	0.10	0.12	0.33

Table 2: Preservation of the modified adiabatic invariant J_{mod}, the modified total energy K, and the difference between the effective frequency $\omega_{eff}(y;\alpha)$ and the "true" frequency $\omega(y)$ under the Verlet discretization.

Let us check if this can be verified numerically (at least) for our simple example from Section 2.

Example (cont.). Almost all necessary ingredients were already given in the previous discussion. We only need an explicit expression for the derivative $b'(q)$. Since the definition of the corresponding conjugate momentum p_y is invariant under the scaling of $b'(q)$ by an arbitrary non-zero expression, we formally define

$$b'(q) \quad = \quad (aq_1^2 + bq_2^2)^{-1/2} \begin{pmatrix} bq_2 \\ -aq_1 \end{pmatrix}$$

which yields

$$b'(q)b'(q)^T \;=\; g'(q)g'(q)^T \;=\omega^2 \quad = \quad \frac{a^2q_1^2 + b^2q_2^2}{aq_1^2 + bq_2^2}\,.$$

Numerical experiments were carried out using the same parameters and initial conditions as in Section 2. The modified adiabatic invariant J_{mod} is given by

$$J_{mod} \quad := \quad \frac{K_x}{\omega_{eff}}\,.$$

The computed results can be found in Table 2 with ΔJ_{mod}, ΔK respectively, replacing ΔJ, ΔH respectively, from Table 1 and

$$\Delta\omega \quad := \quad \max_{t_n\in[0,100]} |\omega(t_n) - \omega_{eff}(t_n)|\,.$$

The numerical results indicate that, for $\alpha \le 1.0$, the Verlet method yields "accurate" solutions to the modified problem with Hamiltonian K. There are a couple of crucial remarks to be made though: First, to leading order in ϵ the (exact) slow motion in the (y, p_y) variable is determined by the reduced Hamiltonian

$$H_{red}(y,p_y) \quad = \quad h(y,p_y) + J\omega(y)\,.$$

Numerically this is replaced by (again to leading order)

$$K_{red}(y, p_y; \alpha) \quad = \quad h(y, p_y) + J_{mod}\omega_{eff}(y; \alpha)$$

which can be $\mathcal{O}(\alpha)$ away from H_{red}! Thus not only the fast solution components are wrongly approximated for $\alpha \sim 1$ but this wrong approximation also effects the slowly varying solution components. Second, it is not obvious that, for $\Delta t \to 0$ and $\alpha = const.$, the solutions obtained from the Verlet method converge to the exact solutions of the modified Hamiltonian K. In fact, we performed the following numerical experiment: For our test example we have $\omega(y) \in [1, \sqrt{2}]$. Thus, the linear stability limit of Verlet implies that we have to take $\alpha \leq \sqrt{2}$. The maximum error in energy for the Verlet method w.r.t. the modified Hamiltonian K was computed for $\alpha \in [0.9, 1.4]$ and $\epsilon = 0.01, 0.02, 0.04$. The results can be found in Fig. 1(a). For $\alpha \geq 1$, the error in energy is quite irregular and does not dependent in an obvious way on α or ϵ (or $\Delta t = \alpha\epsilon$ for that matter). To find out about the source of this behavior, we also did a numerical experiment with $a = b = 2$ which leads to the stiff spring pendulum and $\omega = \sqrt{2}$. See Fig. 1(b). Here a very regular behavior is found. Also the error in the modified energy K decreases for smaller ϵ and fixed α. Note that, according to Mandziuk & Schlick [8], numerically induced resonance instabilities could occur at $\alpha = \sqrt{3}/\sqrt{2}$ (3 : 1 resonance) and $\alpha = 1$ (4 : 1 resonance) which we do not observe for this test problem. Thus, the fluctuations in the energy for the case $a = 2$ and $b = 1$ also seem to be of a different nature. We suspect a bad approximation of the force term $-\nabla_y \omega_{eff}(y; \alpha) J_{mod}$ due to a very low sampling rate for $\alpha \geq 1$ as the source of the problem[7]. As a practical recommendation we suggest that the step-size Δt should be restricted to

$$\Delta t \quad \leq \quad \epsilon\, \omega(y)^{-1}$$

for all y along the numerically computed solutions. This choice insures that at least four integration steps are taken per period of the fast oscillations with frequency ω_{eff}. Fig. 1 also suggests that a larger Δt can be used if $\omega = const.$

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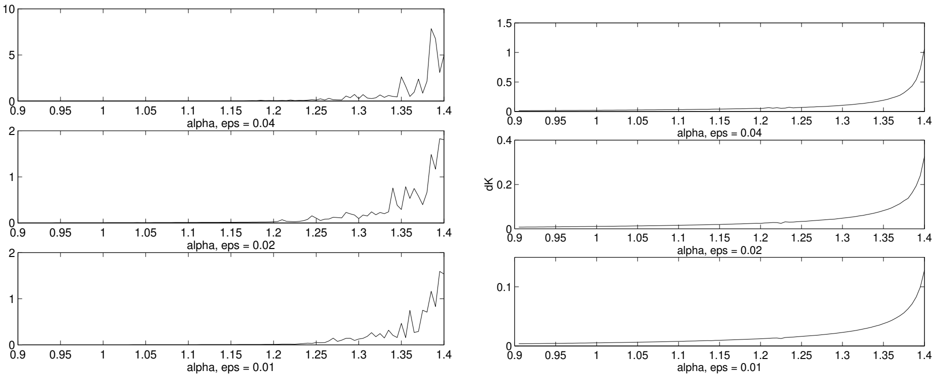

(a) Model problem with $a = 2$ and $b = 1$.

(b) Model problem with $a = 2$ and $b = 2$.

Figure 1: Error in the modified energy function K as a function of α for different values of ϵ.

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