Asymptotic Error Analysis of the Adaptive Verlet Method

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Abstract

The Adaptive Verlet method [7] and variants [6] are time-reversible schemes for treating Hamiltonian systems subject to a Sundman time transformation. These methods have been observed in computer experiments to exhibit superior numerical stability when implemented in a counterintuitive "reciprocal" formulation. Here we give a theoretical explanation of this behavior by examining the leading terms of the modified equation (backward error analysis) and those of the asymptotic error expansion. With this insight we are able to improve the algorithm by simply correcting the starting stepsize.

keywords: Adaptive Verlet method, time-reversible variable stepsizes, Hamiltonian systems, Sundman time-transformations, backward error analysis, asymptotic expansions

1 Introduction

Consider a mechanical Hamiltonian system of the form

$$\frac{d}{dt}q = M^{-1}p, \qquad q(t_0) = q_0, \tag{1}$$

$$\frac{d}{dt}p = F(q), \qquad p(t_0) = p_0, \tag{2}$$

where $q, p \in \mathbf{R}^N$, $M \in \mathbf{R}^{N\times N}$ is a positive definite matrix, and $F = -\nabla_q V$ for some smooth, real-valued potential function V. If different time-scales are present in

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the solution of (1)-(2), an efficient numerical treatment requires variable steps. An alternative approach is to apply a time transformation of the form

$$\frac{dt}{d\tau} = G(q,p),$$

with G a smooth, positive function (also called Sundman transformation) so that, by viewing q and p as functions of the new variable τ, the equations of motion become

$$\frac{d}{d\tau}q = gM^{-1}p, \tag{3}$$

$$\frac{d}{d\tau}p = gF(q), \tag{4}$$

where $g = G(q,p)$. Applying a numerical method with constant stepsize h to (3)-(4) is essentially equivalent to applying the method with stepsize hg_n to (1)-(2). If $G(q,-p) = G(q,p)$, the change of the time variable preserves the reversing symmetry associated to (1)-(2), a property that has been found to be important for recovering realistic qualitative behavior of the original system in numerical simulations [10, 8].

In this article we consider a variant of Verlet's method written in the form

$$q_{n+1/2} = q_n + \frac{h}{2}g_n M^{-1}p_{n+1/2}, \tag{5}$$

$$p_{n+1/2} = p_n + \frac{h}{2}g_n F(q_n), \tag{6}$$

$$q_{n+1} = q_{n+1/2} + \frac{h}{2}g_{n+1} M^{-1}p_{n+1/2}, \tag{7}$$

$$p_{n+1} = p_{n+1/2} + \frac{h}{2}g_{n+1} F(q_{n+1}). \tag{8}$$

Here h represents the fictive timestep (i.e. stepsize in τ), and the indices indicate the timestep. The most obvious choice of g_n is

$$g_n = G(q_n, p_n), \tag{9}$$

which, however, results in an implicit algorithm.

In order to avoid this implicitness, it was suggested in [7] to put $g_0 = G(q_0, p_0)$, and to update the time-scaling factor g from a two-term recurrence relation

$$\Psi(g_n, g_{n+1}, q_n, q_{n+1/2}, q_{n+1}, p_n, p_{n+1/2}, p_{n+1}) = 0$$

with symmetry preserving Ψ. Obviously, the latter equation has to be consistent with the equation $g(\tau_n) = G(q(\tau_n), p(\tau_n))$ in the limit of small h.

A natural choice of Ψ is

$$\Psi = g_{n+1} + g_n - 2G(q_{n+1/2}, p_{n+1/2}), \tag{10}$$

but in experiments this has been found to behave unreliably, particularly in the presence of large forces. A more robust approach is to use the corresponding equation for the reciprocal of g [6],

$$\Psi = \frac{1}{g_{n+1}} + \frac{1}{g_n} - \frac{2}{G(q_{n+1/2}, p_{n+1/2})}. \tag{11}$$

Various semi-explicit and implicit variants of Adaptive Verlet proposed in [7] also use the reciprocal relation. Until now, the reason for this counterintuitive modification of the recurrence relation has not been explained. In Sect. 2, we study for the various methods the leading terms of the modified equation (backward error analysis) and those of the asymptotic error expansions. Each of these has a (nonphysical) oscillating part determined from a certain differential or algebraic equation; a simple analysis of this leading oscillatory term explains the observed differences in stability of the methods. As an outcome of this analysis, we show in Sect. 3 how the oscillations can be attenuated by correcting the starting stepsize.

Another extension of the Verlet scheme to variable stepsizes has recently been proposed independently in [3] and in [9]. In addition to being symmetric, it is a symplectic method, but it has the disadvantage of being implicit in g_{n+1}. A comparison of the different extensions is given in [1].

2 Backward Error Analysis and Asymptotic Expansions

For the choice $g_n = G(q_n, p_n)$, the method is a symmetric one-step method applied to an ordinary differential equation. It is a classical result that the numerical solution can then be formally written as the exact solution of a modified differential equation, and that the global error possesses an expansion in even powers of h (see [5, pp. 555-559] and [4, Sect. II.8]).

We now turn to the more interesting case where g_n is given by a two-term recursion, which allows the algorithm to be completely explicit. The following theorem shows that in this case the numerical solution is a superposition of a smooth function with oscillatory terms. Such a phenomenon is similar to the weak instability of two-step methods (see [4, Sect. III.9]).

Theorem 1 *The numerical solution of the Adaptive Verlet method (5)-(8) can formally be written as*

$$q_n = \widetilde{q}(\tau_n) + (-1)^n \widehat{q}(\tau_n), \quad p_n = \widetilde{p}(\tau_n) + (-1)^n \widehat{p}(\tau_n), \quad g_n = \widetilde{g}(\tau_n) + (-1)^n \widehat{g}(\tau_n), \tag{12}$$

where $\tau_n = nh$ *and*

$$\begin{aligned}
\widetilde{q}\,' &= \widetilde{g} M^{-1} \widetilde{p} + h^2 \widetilde{Q}_2(\cdot) + \dots, & \widehat{q} &= h^2 \widehat{Q}_2(\cdot) + \dots, & (13)\\
\widetilde{p}\,' &= \widetilde{g} F(\widetilde{q}\,) + h^2 \widetilde{P}_2(\cdot) + \dots, & \widehat{p} &= h^2 \widehat{P}_2(\cdot) + \dots, & (14)\\
\widetilde{g} &= G(\widetilde{q}, \widetilde{p}\,) + h^2 \widetilde{G}_2(\cdot) + \dots, & \widehat{g}\,' &= \widehat{G}(\cdot) + h^2 \widehat{G}_2(\cdot) + \dots, & (15)
\end{aligned}$$

with uniquely determined initial values satisfying

$$q_0 = \widetilde{q}(0) + \widehat{q}(0), \qquad p_0 = \widetilde{p}(0) + \widehat{p}(0), \qquad g_0 = \widetilde{g}(0) + \widehat{g}(0). \tag{16}$$

All of the above expansions are formal and in even powers of h. The functions in (13)-(15) depend only on $\widetilde{q}, \widetilde{p}$ and $\widehat{g}$. The functions $\widehat{G}, \widehat{G}_2, \dots$ and also $\widehat{Q}_2, \widehat{P}_2, \dots$ contain $\widehat{g}$ as factor, and $\widehat{g}(0) = \mathcal{O}(h^2)$.

Remark. The right hand side of the differential equation for $\widehat{g}$ (15) contains $\widehat{g}$ as a factor, and $\widehat{g}(0) = \mathcal{O}(h^2)$; these facts imply that $\widehat{g}(\tau) = \mathcal{O}(h^2)$ for τ on compact intervals. Since, the functions $\widehat{Q}_2$ and $\widehat{P}_2$ also contain $\widehat{g}$ as factor, we have in addition $\widehat{q}(\tau) = \mathcal{O}(h^4)$ and $\widehat{p}(\tau) = \mathcal{O}(h^4)$.

Proof. The idea is to insert (12) into the method (5)-(8), to expand, and to compare like powers of h. This computation is significantly simplified if we exploit the symmetric structure of the method and if we expand the resulting expressions around $\tau := \tau_n + h/2$. Neglecting terms of order $\mathcal{O}(h^4)$ and those of the form $\mathcal{O}(h^2\widehat{q})$, $\mathcal{O}(h^2\widehat{p})$, $\mathcal{O}(\widehat{q}^{\,2})$, $\mathcal{O}(\widehat{q}\,\widehat{p})$, $\mathcal{O}(\widehat{p}^{\,2})$) and omitting the obvious argument τ, we get

$$\begin{aligned}
\frac{1}{2}(p_{n+1}+p_n) &= \widetilde{p} + \frac{h^2}{8}\widetilde{p}\,'' - (-1)^n \frac{h}{2}\widehat{p}\,' + \ldots \\
\frac{h}{4}(g_n - g_{n+1}) &= -\frac{h^2}{4}\widetilde{g}\,' + (-1)^n\Big(\frac{h}{2}\widehat{g} + \frac{h^3}{16}\widehat{g}\,''\Big) + \ldots\ .
\end{aligned}$$

Using these and similar relations for other variables, we obtain for the intermediate approximations $q_{n+1/2}$ and $p_{n+1/2}$ the expansions

$$\begin{aligned}
p_{n+1/2} &= \frac{1}{2}(p_{n+1}+p_n) + \frac{h}{4}\Big(g_nF(q_n) - g_{n+1}F(q_{n+1})\Big) \\
&= \widetilde{p} + \frac{h^2}{8}\Big(\widetilde{p}\,'' - 2(\widetilde{g}\,F(\widetilde{q}\,))'\Big) && (17) \\
&\quad -(-1)^n\frac{h}{2}\Big(\widehat{p}\,' - \widehat{g}F(\widetilde{q}\,) - \widetilde{g}F_q(\widetilde{q}\,)\widehat{q}\Big) + (-1)^n\frac{h^3}{16}(\widehat{g}F(\widetilde{q}\,))'' + \ldots\ , \\
q_{n+1/2} &= \frac{1}{2}(q_{n+1}+q_n) + \frac{h}{4}(g_n - g_{n+1})M^{-1}p_{n+1/2} \\
&= \widetilde{q} + \frac{h^2}{8}\Big(\widetilde{q}\,'' - 2\widetilde{g}\,'M^{-1}\widetilde{p} + 2\widehat{g}^{\,2}M^{-1}F(\widetilde{q}\,)\Big) - (-1)^n\frac{h}{2}\Big(\widehat{q}\,' - \widehat{g}M^{-1}\widetilde{p}\Big) && (18) \\
&\quad +(-1)^n\frac{h^3}{16}\Big(\widehat{g}M^{-1}\widetilde{p}\,'' + \widehat{g}\,''M^{-1}\widetilde{p} - 2\widehat{g}(\widetilde{g}\,M^{-1}F(\widetilde{q}\,))' \\
&\qquad\qquad -2\widehat{g}\,\widetilde{g}\,'M^{-1}F(\widetilde{q}\,)\Big) + \ldots\ ,
\end{aligned}$$

where $F_q(q)$ denotes the derivative of F with repect to q, and $'$ denotes the derivative with respect to τ. We now write the main formulas of the method (with the choice (10) for g_n) as

$$q_{n+1} - q_n = \frac{h}{2}(g_n + g_{n+1})M^{-1}p_{n+1/2}\ , \tag{19}$$

$$p_{n+1} - p_n = \frac{h}{2}\Big(g_nF(q_n) + g_{n+1}F(q_{n+1})\Big)\ , \tag{20}$$

$$\frac{1}{2}(g_{n+1} + g_n) = G(q_{n+1/2}, p_{n+1/2}). \tag{21}$$

Inserting the relations (12) and (17)-(18), we get

$$h\widetilde{q}\,' + \frac{h^3}{24}\widetilde{q}\,''' - (-1)^n 2\,\widehat{q} + \dots \tag{22}$$
$$= h\Big(\widetilde{g} + \frac{h^2}{8}\widetilde{g}\,'' - (-1)^n\frac{h}{2}\widehat{g}\,'\Big)M^{-1}\Big(\widetilde{p} + \frac{h^2}{8}(\widetilde{p}\,'' - 2(\widetilde{g}\,F(\widetilde{q}\,))') + (-1)^n\frac{h}{2}\widehat{g}F(\widetilde{q}\,)\Big) + \dots\ ,$$

$$h\widetilde{p}\,' + \frac{h^3}{24}\widetilde{p}\,''' - (-1)^n 2\,\widehat{p} + \dots \tag{23}$$
$$= h\Big(\widetilde{g}F(\widetilde{q}\,) + \widehat{g}F_q(\widetilde{q}\,)\widehat{q}\Big) + \frac{h^3}{8}(\widetilde{g}F(\widetilde{q}\,))'' - (-1)^n\frac{h^2}{2}(\widehat{g}F(\widetilde{q}\,))' + \dots\ ,$$

$$\widetilde{g} + \frac{h^2}{8}\widetilde{g}\,'' - (-1)^n\frac{h}{2}\widehat{g}\,' - (-1)^n\frac{h^3}{48}\widehat{g}\,''' + \dots \tag{24}$$
$$= G(\widetilde{q},\widetilde{p}\,) + G_q(\widetilde{q},\widetilde{p}\,)(q_{n+1/2} - \widetilde{q}\,) + G_p(\widetilde{q},\widetilde{p}\,)(p_{n+1/2} - \widetilde{p}\,) + \dots\ ,$$

where G_q and G_p denote partial derivatives. Comparing the non-oscillating and oscillating parts in (22)-(24) yields equations for $\widetilde{q}\,',\widetilde{p}\,',\widetilde{g}$ and $\widehat{q},\widehat{p},\widehat{g}\,'$, respectively. The higher derivatives appearing in the right-hand side have to be eliminated iteratively. This gives the modified equations (13)-(15). We obtain for example

$$\widehat{G}(\widetilde{q},\widetilde{p},\widehat{g}\,) = -\widehat{g}\Big(G_q(\widetilde{q},\widetilde{p}\,)M^{-1}\widetilde{p} + G_p(\widetilde{q},\widetilde{p}\,)F(\widetilde{q}\,)\Big). \tag{25}$$

The algebraic relations for $\widehat{q},\widehat{p},\widetilde{g}$ in (13)-(15) together with (16) constitute a set of six equations for the unknowns $\widetilde{q}(0),\widehat{q}(0),\widetilde{p}(0),\widehat{p}(0),\widetilde{g}(0),\widehat{g}(0)$. By the implicit function theorem they have a unique solution close to $(q_0,0,p_0,0,g_0,0)$,which can be written as a formal series in powers of h^2. □

Remark. For the choice (11) only the equations (21) and (24) have to be adapted, and one gets

$$\widehat{G}(\widetilde{q},\widetilde{p},\widehat{g}\,) = +\widehat{g}\Big(G_q(\widetilde{q},\widetilde{p}\,)M^{-1}\widetilde{p} + G_p(\widetilde{q},\widetilde{p}\,)F(\widetilde{q}\,)\Big), \tag{26}$$

instead of (25). For the more general situation

$$\frac{1}{2}\Big(L(g_{n+1}) + L(g_n)\Big) = L\Big(G(q_{n+1/2},p_{n+1/2})\Big),$$

which includes (10) and (11) as special cases, we get

$$\widehat{G}(\widetilde{q},\widetilde{p},\widehat{g}\,) = -\widehat{g}\Big(1 + \frac{L_{gg}(\widetilde{g}\,)\widetilde{g}}{L_g(\widetilde{g}\,)}\Big)\Big(G_q(\widetilde{q},\widetilde{p}\,)M^{-1}\widetilde{p} + G_p(\widetilde{q},\widetilde{p}\,)F(\widetilde{q}\,)\Big). \tag{27}$$

Corollary 2 (Asymptotic Expansions) *The functions $\widetilde{q}(\tau)$, $\widehat{q}(\tau)$, $\widetilde{p}(\tau)$, $\widehat{p}(\tau)$, $\widetilde{g}(\tau)$, $\widehat{g}(\tau)$ of Theorem 1 all have asymptotic expansions in even powers of h. In particular,*

$$\widetilde{g}(\tau) = g(\tau) + h^2 g_2(\tau) + \mathcal{O}(h^4), \qquad \widehat{g}(\tau) = h^2\widehat{g}_2(\tau) + h^4\widehat{g}_4(\tau) + \mathcal{O}(h^6), \tag{28}$$

where $g(\tau) = G(q(\tau),p(\tau))$ with $(q(\tau),p(\tau))$ the solution of (3)-(4).

For the choice (10) of g_n with $G(q)$ only depending on q,

$$\widehat{g}_2(\tau) = \frac{G(q_0)^2}{8g(\tau)}\Big(G(q_0)G_{qq}(q_0)(M^{-1}p_0, M^{-1}p_0) + 2(G_q(q_0)M^{-1}p_0)^2\Big), \tag{29}$$

and for the choice (11) we have:

$$\widehat{g}_2(\tau) = \frac{g(\tau)}{8}\, G(q_0)G_{qq}(q_0)(M^{-1}p_0, M^{-1}p_0). \tag{30}$$

Proof. We insert the formulas (28) and similar equations for $\widetilde{q}(\tau)$, $\widehat{q}(\tau)$, $\widetilde{p}(\tau)$, $\widehat{p}(\tau)$ into the modified differential-algebraic system (13)-(15), then compare like powers of h. This yields differential equations for $\widetilde{q}_{2i}(\tau)$, $\widetilde{p}_{2i}(\tau)$, $\widehat{g}_{2i}(\tau)$, and algebraic relations for $\widehat{q}_{2i}(\tau)$, $\widehat{p}_{2i}(\tau)$, $\widetilde{g}_{2i}(\tau)$. A straightforward computation gives (for (10)):

$$\begin{aligned} g_2(\tau) &= -\frac{1}{8}g''(\tau) + G_q(q(\tau),p(\tau))\Big(\frac{1}{8}q''(\tau) + q_2(\tau) - \frac{1}{4}g'(\tau)M^{-1}p(\tau)\Big) \\ &\qquad + G_p(q(\tau),p(\tau))\Big(p_2(\tau) - \frac{1}{8}p''(\tau)\Big)\ , \qquad (31) \\ \widehat{g}_2{}'(\tau) &= -\widehat{g}_2(\tau)g'(\tau)/g(\tau). \qquad (32) \end{aligned}$$

The differential equation (32) can be solved for $\widehat{g}_2(\tau)$, and we obtain $\widehat{g}_2(\tau)g(\tau) = \widehat{g}_2(0)g(0)$. Since $q_2(0) = p_2(0) = 0$, we get $g_2(0)$ from (31) and then $\widehat{g}_2(0)$ from (16). This yields the formula (29) for $\widehat{g}_2(\tau)$. Formula (30) is obtained in the same way. □

Example 1 For an illustration of the oscillatory terms in the numerical solution and in the stepsizes we consider the problem

$$q' = p, \qquad p' = -1/q^2, \qquad G(q) = q^2\ ,$$

with initial values $q_0 = 1, p_0 = -2$. We apply the adaptive Verlet method with fictive stepsize $h = 0.08$. The picture on the left in Fig. 1 shows the values of g_n as a function of the time t_n, (i) for the choice (10) (indicated by small circles), and (ii) for the choice (11) (small squares). The second and third pictures of Fig. 1 show the values $g_n - g(t_n)$ together with the smooth curves $\pm h^2\widehat{g}_2(t)$. For the choice (10) we observe increasing oscillations, and for $t \geq 0.22$ the numerical solution becomes meaningless and the stepsizes hg_n even become negative. We have joined consecutive points of $\{g_n\}$ by a polygon in order to better illustrate this phenomenon. For the choice (11) the oscillations are very small (they can be observed only in the scale of the third picture) and they are decreasing. This can be explained by the fact that $\widehat{g}_2(t)$ is inversely proportional to $g(t)$ for the choice (10), whereas it is proportional to $g(t)$ for the choice (11), and $g(t) = q(t)^2$ is approaching zero. The second and third pictures show excellent agreement of g_n with the expansion $g(t_n) + h^2 g_2(t_n) + (-1)^n h^2 \widehat{g}_2(t_n) + \mathcal{O}(h^4)$, even for the rather large value $h = 0.08$ (observe that in the last two pictures the term $h^2 g_2(t)$ is not included in the smooth function).

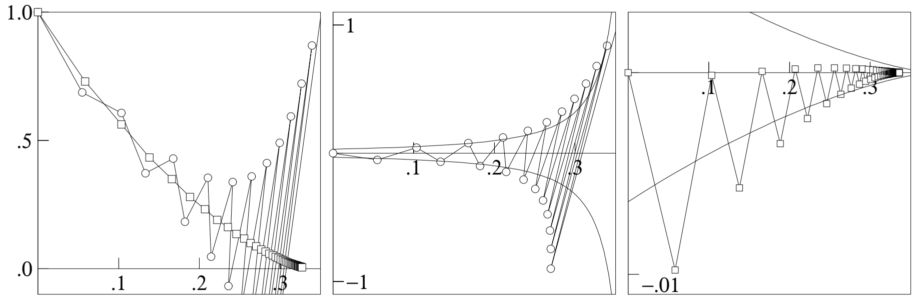

Figure 1: The values of g_n (left picture) and $g_n - g(t_n)$ (second and third pictures) as a function of time t_n; circles indicate the results for the choice (10), and squares for the choice (11).

3 Elimination of the Dominant Oscillatory Terms

In the proof of Corollary 2, we have seen that the function $\widehat{g}_2(\tau)$ is the solution of a linear autonomous differential equation. If we are able to achieve $\widehat{g}_2(0) = 0$, the function $\widehat{g}_2(\tau)$ will remain zero for all τ and the dominant term in $\widehat{g}(\tau)$ will be eliminated, implying $\widehat{g}(\tau) = \mathcal{O}(h^4)$. Since $\widehat{g}$ is a factor in the algebraic relations (13)-(14) for $\widehat{q}$ and $\widehat{p}$, this will also imply that $\widehat{q}(\tau) = \mathcal{O}(h^6)$ and $\widehat{p}(\tau) = \mathcal{O}(h^6)$.

The idea is to use

$$g_0 = G(q_0, p_0) + \alpha_2 h^2 + \alpha_4 h^4 + \dots \tag{33}$$

for the initial stepsize instead of $g_0 = G(q_0, p_0)$. Such a choice neither affects the modified differential-algebraic system (13)-(15) nor the relations (16) for its initial values. If (33) is an expansion in even powers of h, the symmetry of the method will not be destroyed. If g_0 is computed from (33), the value of $\widehat{g}_2(0)$ is given by

$$\alpha_2 = g_2(0) + \widehat{g}_2(0).$$

Therefore, the choice $\alpha_2 = g_2(0)$ with $g_2(0)$ given by (31) implies $\widehat{g}_2(0) = 0$.

Example 2 For the problem of Example 1 it is not difficult to compute $g_2(0)$ from (31). We have $g_2(0) = -5$ for the choice (10) and $g_2(0) = -1$ for (11). With the same fictive stepsize $h = 0.08$ and with the same initial values as before we apply the adaptive Verlet scheme, but we use $g_0 = G(q_0) + h^2 g_2(0)$ instead of $g_0 = G(q_0)$. The result is shown in Fig. 2. The values of g_n (first picture) and $g_n - g(t_n)$ for the choice (10) (second picture) still show an oscillating behaviour, but the magnitude of the oscillations is smaller and proportional to h^4. For the choice (11) (small squares) the oscillations are completely eliminated.

For general problems, the computation of the value $g_2(0)$ with the help of a formula like (31) can be cumbersome, in particular if G also depends on p. It is of course possible to use automatic differentiation [2]. Another possibility is to apply the adaptive Verlet scheme with $g_0 = G(q_0, p_0)$ two steps with positive fictive stepsize

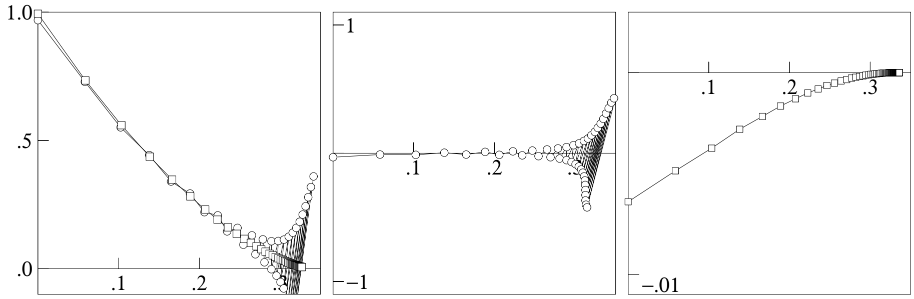

Figure 2: The same interpretation as in Fig. 1, but with $g_0 = G(q_0) + h^2 g_2(0)$ instead of $g_0 = G(q_0)$.

η and two steps with $-\eta$ (for η something like $\eta \approx eps^{1/4}$, where eps is the machine precision, the roundoff and truncation errors are of the same order). From the values $g_{-2}, g_{-1}, g_0, g_1, g_2$, obtained in this way, we then compute the fourth central difference

$$\delta_4 = g_{-2} - 4g_{-1} + 6g_0 - 4g_1 + g_2,$$

which eliminates the smooth terms up to order four and yields $\delta_4 = 16\eta^2 \widehat{g}_2(0) + \mathcal{O}(\eta^4)$. With the starting stepsize

$$g_0 = G(q_0, p_0) - \frac{h^2}{16\,\eta^2}\,\delta_4 \tag{34}$$

we therefore eliminate the dominant oscillatory terms. We repeated the numerical experiment of Example 2 with g_0 from (34) and observed the same effect as with $g_0 = G(q_0) + h^2 g_2(0)$.

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