Symplectic integrators with adaptive time steps

A S Richardson¹ and J M Finn²

¹ Pulsed Power Physics Branch, Plasma Physics Division, Naval Research Laboratory, Washington, DC, USA
² T-5, Applied Mathematics and Plasma Physics, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

E-mail: steve.richardson@nrl.navy.mil and finn@lanl.gov

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Abstract
In recent decades, there have been many attempts to construct symplectic integrators with variable time steps, with rather disappointing results. In this paper, we identify the causes for this lack of performance, and find that they fall into two categories. In the first, the time step is considered a function of time alone, $\Delta = \Delta(t)$. In this case, backward error analysis shows that while the algorithms remain symplectic, parametric instabilities may arise because of resonance between oscillations of $\Delta(t)$ and the orbital motion. In the second category the time step is a function of phase space variables $\Delta = \Delta(q, p)$. In this case, the system of equations to be solved is analyzed by introducing a new time variable $\tau$ with $dt = \Delta(q, p) d\tau$. The transformed equations are no longer in Hamiltonian form, and thus do not benefit from integration methods which would be symplectic for Hamiltonian systems. We analyze two methods for integrating the transformed equations which do, however, preserve the structure of the original equations. The first is an extended phase space method, which has been successfully used in previous studies of adaptive time step symplectic integrators. The second, novel, method is based on a non-canonical mixed-variable generating function. Numerical trials for both of these methods show good results, without parametric instabilities or spurious growth or damping. It is then shown how to adapt the time step to an error estimate found by backward error analysis, in order to optimize the time-stepping scheme. Numerical results are obtained using this formulation and compared with other time-stepping schemes for the extended phase space symplectic method.

(Some figures may appear in colour only in the online journal)

1. Introduction

Adaptive time integration schemes for ODEs are well established and perform extremely well for many applications. However, for applications involving the integration of Hamiltonian systems, there are good reasons for using symplectic integrators [1]. This is particularly true in applications such as accelerators, in which very long orbits must be integrated. Symplectic integrators are also used in particle-in-cell (PIC) codes for plasma applications, where for economy integrators with lower order of accuracy must be used, but it is important that the Hamiltonian phase space structure be preserved. The same is true for molecular dynamics codes [2, 3], which are of use for dense plasmas as well as other applications. Similarly, for tracing magnetic field lines (e.g. in tokamaks or reversed field pinches) or doing RF (radio frequency) ray tracing, symplectic integrators can be very useful. Further, variational integrators (very closely related to symplectic integrators, but where the Lagrangian is discretized and variational equations are formed with it) have been used to integrate guiding center orbits in non-canonical variables [4]. To the best of our knowledge, the symplectic integrators in use for plasma and particle beam applications all have uniform time-stepping. However, for these applications there are situations in which variable or adaptive time stepping could increase efficiency greatly. For example, in accelerators, particles can experience fields that vary over a wide range of length scales. The same is true for PIC and MD codes, for example, for particles moving in and out of shocks or magnetic reconnection layers, or undergoing close collisions.
There have been studies of symplectic integrators with variable time steps, but the early results were not promising [5–11]. Among these studies, there have been two types of variation of time steps. In the first set of studies, the time step varies with time explicitly, and in some cases varies from $\Delta t = \Delta t_1$ to $\Delta t = \Delta t_2$ on alternate blocks of time steps. In these studies problems were observed to arise. In the second set of studies, the time step was chosen with $\Delta t = \Delta(t)$, where $q$, $p$ are the dynamical variables. For any adaptive scheme for an autonomous system of equations, the time step is of this form. For the $\Delta(t)$ case, the equations are no longer in canonical Hamiltonian form (but may be Hamiltonian in non-canonical variables; see below) and indeed unfavorable results are found. The disappointing results for both of these cases have contributed to the general impression that if you need an adaptive time step integrator, you are better served using a high order non-symplectic integration method3.

In this paper, we take a new look at symplectic integrators with adaptive time stepping. Our focus is not on developing the most efficient or accurate symplectic integrators, but to understand and solve the problems that have been encountered in using symplectic integrators with variable time steps, and to outline a method of obtaining an optimal time-step adaptation scheme.

In section 2 we start by considering time steps depending explicitly on time alone as $\Delta t = \Delta(t) = \Delta_0(1 + \epsilon \cos \omega t)$. In section 2.1 we consider several examples of first and second order symplectic integrators applied to the harmonic oscillator, and apply modified equation analysis or backward error analysis [12, 13, 15, 16]. This allows us to find the modified Hamiltonian system which the integration scheme, including the effect of numerical errors, actually solves. From this analysis we find that resonances between $\omega$ and the oscillator frequency $\Omega_0$ drive parametric instabilities. The resonances have $\omega = m\Omega_0$, the lowest order resonance having $m = 2$. For first order schemes the resonance width scales as $\epsilon \Delta_0$, while second order schemes have width $\propto \epsilon^2 \Delta_0^2$. These parametric instabilities explain the problematic results obtained in the papers dealing with $\Delta = \Delta(t)$ [6, 8–10]. In the context of the harmonic oscillator, these problems were identified as arising from parametric instabilities by Piché [17].

We continue in section 2.2 by numerically investigating time step variations $\Delta(t) = \Delta_0(1 + \epsilon \cos \omega t)$, by integrating the harmonic oscillator with a symplectic method. We find parametric instabilities with resonance widths as predicted by the modified equation analysis. We show results of numerical integrations of a cubic oscillator with the nonlinear potential $V(q) = q^2/2 + q^3/3$, in which the frequency varies with respect to the action variable, $\Omega = \Omega(J)$. The parametric instabilities seen globally for the harmonic oscillator show up as nonlinear resonances or islands, where $\omega = m\Omega(J)$, with $m$ depending on the integration method and the Hamiltonian being integrated. We observed $m = 1$ islands for the cubic oscillator, integrated with the Crank–Nicolson (CN) method. The calculations of this section illustrate the point that, when considering $\Delta = \Delta(t)$, problems arise because the equations being solved become unstable (but still Hamiltonian), and not because the integration scheme fails to be symplectic.

In section 3 we study time step variations $\Delta = \Delta(q, p)$. With $\Delta(q, p) \propto 1/\rho(q, p)$, the straightforward substitution $\rho(q, p)\, dt = d\tau$ leads to equations (having $\tau$ as the independent variable) that are not Hamiltonian equations in canonical form. Integrators which are symplectic for Hamiltonian systems are therefore not expected to have the benefits of symplectic integrators when applied to these modified equations, and again it has been observed that they do not. In section 3.1 we review one approach to solving this problem, by extending the phase space $(q, p) \rightarrow (q, q_0, p, p_0)$, where $q_0 = t$ and $p_0$ is its conjugate momentum. After this transformation to an extended phase space, it is easily shown that the resulting equations are Hamiltonian in canonical form and can be integrated by any fixed time step ($\Delta t = h = \text{const}$) symplectic integrator in this extended phase space. This is a well-known method, and has been used to obtain symplectic integration schemes with variable time steps by Hairer [12], and also Reich [13]. Hairer described this approach as a ‘meta-algorithm’ because any symplectic integrator can be used in the extended phase space. We then present numerical results in section 3.2 for the cubic oscillator (with two different symplectic integrators) which show that, even with a step size variation that appears to have an $m = 1$ resonance, evidence of non-symplectic behavior occurs and no resonant islands indicative of parametric instability form.

In section 3.3 we introduce a second method for dealing with the problems that arise when $\Delta = \Delta(q, p)$. The point of introducing a second method is to illustrate that the main problem with $\Delta(q, p)$ is that the equations are no longer Hamiltonian, and that there are potentially many ways to address this problem. The extended phase space method ‘fixes’ the equations by embedding them in a higher dimensional Hamiltonian system. This alternative approach does not extend the dimension of the phase space, but rather recognizes the fact that, with $\tau$ as the independent variable and $\rho(q, p)\, dt = d\tau$, the equations are Hamiltonian equations in non-canonical variables [18]. (This is true only for one degree of freedom, i.e. 2D phase space.) That is, the equations can be expressed in terms of a non-canonical bracket [18]. We write the non-canonical variables as $(x, y)$ with the numerical scheme giving the mapping $(x, y) = (x(\tau), y(\tau)) \rightarrow (X, Y) = (x(\tau + h), y(\tau + h))$. Equivalent to the non-canonical bracket, the fundamental two-form is $\rho(x, y)\, dx \wedge dy$ rather than the canonical form $dq \wedge dp$. We describe a method for constructing a non-canonical generating function $F(x, y)$ which gives a map $T_F(h)$ that is a first order accurate integrator preserving the two-form. We discuss its relation with transforming to canonical variables (guaranteed to be possible by the Darboux theorem [18]). We then find a complementary non-canonical generating function $G(X, Y)$ which leads to another non-canonical map $T_G(h)$, which is also first order accurate and preserves the two-form. Maps preserving the two-form

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3 An exception to this is the extended phase space approach of Hairer [12] and Reich [13], which we discuss in later sections. Some authors [14] also suggest that methods which are reversible under some symmetry $R(\text{RT}(h)R = T(h))^{-1}$, where the one-time-step map is $T(h)$ and $R$ is an involution, $R^2 = 1$ should be considered in place of symplectic integrators. We do not consider reversible methods here because their advantages are limited to systems where the original flow also has this symmetry property.
\[ \rho(x, y) \, dx \wedge dy \text{ are called Poisson integrators [19–22]} \] and conserve the measure \( \int \rho \, dx \, dy \) rather than the area \( \int dq \, dp \).

We show that \( T_f(h)^{-1} = T_f(-h) \) and vice versa, so that the composition \( T(h) = T_f(h/2) \circ T_f(h/2) \) is time symmetric \( (T(h)^{-1} = T(h)) \) and therefore second order accurate. Finally, we show numerical results in section 3.4 using the composed map \( T(h) \), applied to the cubic oscillator. As with the extended phase space method, this method is stable, with errors in the energy remaining bounded.

In section 4 we study the choice of time step variation \( \rho(q, p) \). We begin by using backward error analysis for a slightly different purpose than in section 2, namely to estimate the form of the error of an integrator, and then devise a scheme to minimize the total error. This scheme takes the form of an equidistribution principle, of the form \( \rho_{\text{exp}}(q, p) \, dt = \Omega(t) \), with uniform steps in \( \tau \).

We then compare the error in numerical integration using \( \rho_{\text{exp}} \) to the error obtained for fixed time steps, to the error obtained for time steps designed to give equal arc length per step, and to step tuning using a weighted average of \( \rho_{\text{exp}} \) and \( \rho = 1 \). We show numerical results showing that, among these options for time step variation, \( \rho_{\text{exp}} \) does indeed minimize the total error.

In section 5 we summarize our work. In appendix A we consider the relationship between the cases with \( \Delta(t) \) and \( \Delta(q, p) \). We show that, while a simple argument motivates the use of \( \Delta(t) \), this is only valid for short times. We explain how this is analogous to the problems which arise in perturbation theory, where a perturbation causes a frequency shift, but at lowest order it appears a secularity or an instability. In appendix B we review non-canonical variables, brackets, and forms, material necessary for section 3.3.

2. Integration with variable time step \( \Delta(t) \)

In this section we will investigate symplectic integrators with a variable time step \( \Delta = \Delta(t) \), in order to understand better the results that have been obtained in the literature. Using modified equation analysis, we will see that the problems that have been reported are best understood as a parametric instability due to resonance between the system dynamics and the time dependence of \( \Delta(t) \).

2.1. Modified equation analysis and parametric instabilities

We first look at the Harmonic oscillator \( H = p^2/2 + \Omega_0^2q^2/2 \). With the change of variables \( p \rightarrow p/\sqrt{\Omega_0} \) and \( q \rightarrow \sqrt{\Omega_0}q \) we obtain \( H = \Omega_0(p^2 + q^2)/2 \). The leapfrog (LF) method, which is first order accurate when \( q \) and \( p \) are not taken to be staggered, with \( \Delta = \Delta(t) \) gives

\[
q_{i+1} = q_i + \Delta(t)\Omega_0 p_i, \quad \text{(1)}
\]

\[
p_{i+1} = p_i - \Delta(t)\Omega_0 q_i, \quad \text{(2)}
\]

Modified equation analysis begins by expanding \( q_{i+1} = q_i + \Delta(t)\dot{q}_i + \Delta(t)^2\ddot{q}_i/2 + \cdots \) and similarly for \( p_{i+1} \). We obtain

\[
\dot{q} = \frac{\Delta(t)^2}{2} q + \Omega_0 p + O(\Delta^2), \quad \text{(3)}
\]

\[
\dot{p} = -\Omega_0 q - \frac{\Delta(t)^2}{2} p + O(\Delta^2). \quad \text{(4)}
\]

Figure 1 shows this predicted region of instability as a function of \( \omega \) and \( \epsilon \). Numerical results for comparison are shown in the next section. Carrying out this analysis to one higher order in \( \Delta_0 \) gives an \( O(\Delta_0^2) \) correction to the \( \phi \)- and time-independent

\[
H' = \frac{\Omega_0}{2} (p^2 + q^2) + \frac{\Delta(t)^2}{2} q p. \quad \text{(5)}
\]

As expected, the modified equations are in Hamiltonian form [13, 16, 23–26]. With the action-angle transformation \( q = \sqrt{2J} \cos \phi \), \( p = -\sqrt{2J} \sin \phi \) and setting \( \Delta(t) = \Delta_0 (1 + \epsilon \cos \omega t) \) we obtain

\[
H' = \Omega_0 J \left( 1 - \frac{\Omega_0 \Delta_0}{2} \sin 2\phi \right) - \frac{\Omega_0^2 \Delta_0 \epsilon}{4} J [\sin (2\phi - \omega t) + \sin (2\phi + \omega t)]. \quad \text{(6)}
\]

Keeping only the resonant \( O(\Delta_0) \) term \( \propto \sin (2\phi - \omega t) \), we obtain

\[
H' \approx \Omega_0 J - \frac{\Omega_0^2 \Delta_0 \epsilon}{4} \sin (2\phi - \omega t). \quad \text{(7)}
\]

The canonical transformation \( \psi = \phi - \omega t/2 \), \( K' = H' - \omega J/2 \) (J unchanged) transforms to a rotating frame in phase space and gives

\[
K' = \left( \Omega_0 - \frac{\omega}{2} \right) J - \frac{\Omega_0^2 \Delta_0 \epsilon}{4} J \sin 2\psi. \quad \text{(8)}
\]

We conclude from this backward error analysis that the harmonic oscillator with time step \( \Delta(t) = \Delta_0 (1 + \epsilon \cos \omega t) \) is unstable if

\[
\left| \Omega_0 - \frac{\omega}{2} \right| < \frac{\Omega_0^2 \Delta_0 \epsilon}{4}, \quad \text{(9)}
\]

since \( K' \) is hyperbolic in this case. This instability is a parametric instability associated with the resonance \( \omega = 2\Omega_0 \). Figure 1 shows this predicted region of instability as a function of \( \omega \) and \( \epsilon \). Numerical results for comparison are shown in the next section. Carrying out this analysis to one higher order in \( \Delta_0 \) gives an \( O(\Delta_0^2) \) correction to the \( \phi \)- and time-independent
terms in $K'$, which gives rise to a positive $O(\Delta^3)$ shift in the resonant frequency independent of $\epsilon$, discussed in the next section.

Another integration scheme is symmetrized leapfrog, which is second order accurate, and takes the form

$$q_{i+1} = q_i + \frac{\Delta(t_i)\Omega_0}{2}p_i,$$

$$p_{i+1} = p_i - \frac{\Delta(t_i)\Omega_0q_i}{2},$$

$$(10)$$

This leads to a modified equation

$$\dot{q} = \Omega_0 p - \frac{\Delta(t)^2\Omega_0^3}{12} p, \quad \dot{p} = -\Omega_0 q - \frac{\Delta(t)^2\Omega_0^3}{2} q,$$  

with modified Hamiltonian

$$H' = \Omega_0 \left(1 - \frac{\Delta(t)^2\Omega_0^3}{12} \right)p^2 + \Omega_0 \left(1 + \frac{\Delta(t)^2\Omega_0^3}{6} \right)q^2.$$  

(12)

A similar analysis to that above for first order LF leads to

$$K' = \left( \Omega_0 + \frac{\Omega_0^3\Delta^2_0}{24} - \frac{\omega}{2} \right)J + \frac{\Omega_0^3\Delta^2_0}{8} J \cos 2\psi.$$  

(13)

Note that for this method, the frequency shift enters at the same order as the resonant term. We conclude that parametric instability occurs for

$$\left| \Omega_0 + \frac{\Omega_0^3\Delta^2_0}{24} \right| < \frac{\Omega_0^3\Delta^2_0}{8}.$$  

(14)

This instability is centered around $\omega = m(\Omega_0 + \Omega_0^3\Delta^2_0/24)$, again with $m = 2$, but in a narrower range $\sim \epsilon \Delta^2_0$. (Resonances with other values of $m$ enter at higher order in $\Delta_0$ and $\epsilon$.) Also note that, because the frequency shift enters at the same order as the resonant term, the shift is comparable to the resonance width for $\epsilon \sim 1$.

As another second order accurate example, we consider CN,

$$q_{i+1} = q_i + h(t_i)\Omega_0 \frac{p_i + p_{i+1}}{2},$$

$$p_{i+1} = p_i - h(t_i)\Omega_0 \frac{q_i + q_{i+1}}{2},$$

(15)

for which the modified equation analysis gives

$$\dot{q} = \left(1 - \frac{\Delta(t)^2\Omega_0^3}{12} \right)\Omega_0 p, \quad \dot{p} = -\left(1 - \frac{\Delta(t)^2\Omega_0^3}{12} \right)\Omega_0 q,$$

or

$$H' = \left(1 - \frac{\Delta(t)^2\Omega_0^3}{12} \right)\Omega_0 \left(\frac{p^2 + q^2}{2} \right) = \Omega(t) J.$$  

(16)

Here, $H'$ is independent of $\phi$ and the action $J = (p^2 + q^2)/2$ is an invariant to order $\Delta^2$, and the errors are all in the phase $\phi$: the frequency $\Omega(t) = 1 - \Delta(t)^2\Omega_0^2/12$ is downshifted for this case. We conclude that parametric instabilities cannot occur to this order for CN. It is easily seen that CN preserves the action $J$ exactly for the harmonic oscillator; this shows that we have $H' = \Omega(t)(p^2 + q^2)/2$ to all orders. Further, the explicit time dependence disappears if we introduce $\tau$ such that $\Omega(t) dt = d\tau$.

2.2. Numerical results with $\Delta = \Delta(t)$

The parametric resonances described for the harmonic oscillator in the previous section were studied numerically, and the results are shown in figures 1 and 2. Figure 1 shows the numerical results, using the first order LF method, again with time steps given by $\Delta(t) = \Delta_0(1 + \epsilon \cos \omega t)$. The red lines show the boundaries of the unstable region in $\omega$, $\epsilon$ parameter space, as predicted in equation (9). The colors show the logarithm of the value of the Hamiltonian at the end ($t = 300$) of a numerically computed orbit. For unstable parameter values, the orbit spirals outward, and the final value of the Hamiltonian becomes exponentially large. The numerically computed region of instability agrees well with the prediction of equation (9), and also shows the $O(\Delta^2)$ offset in frequency $\epsilon = 0$. In figure 2 we examine how, for parameters where the integration is unstable, a circle of initial conditions is stretched out into a long thin ellipse. Since the LF method is still symplectic, the area of the ellipses is preserved.

As described above, first order LF integration of the harmonic oscillator with variable time step $\Delta(t) = \Delta_0(1 + \epsilon \cos \omega t)$ was found to be unstable near the resonance $\omega = 2\Omega_0$. For a nonlinear oscillator, the oscillation frequency $\Omega_0$ depends on the amplitude. We thus expect that the numerical integration of a nonlinear oscillator would exhibit resonant islands, rather than exhibiting global parametric instability.

For example, consider a Hamiltonian with a cubic potential

$$H(q, p) = \frac{q^2 + p^2}{2} + \frac{q^3}{3}.$$  

(18)

This Hamiltonian has an $O$-point at $(q, p) = (0, 0)$ and an $X$-point at $(-1, 0)$. Inside the separatrix of the X-point, this system exhibits nonlinear oscillations. For this system and first order LF, the time step variation $\Delta(t) = \Delta_0(1 + \epsilon \cos \omega t)$ introduces an $m = 1$ resonance ($\omega = \Omega_0$), which is readily
understood by backward error analysis. Specifically, this analysis gives a term in the modified Hamiltonian which is proportional to \( \sin \phi \cos \omega t \), which leads to the \( m = 1 \) resonance, a term proportional to \( \sin(\phi - \omega t) \).

Figure 3 shows the results of integrating this system with the CN method, and the same time steps variation. The frequency \( \omega_0 \), \( 0 < \omega < 1 \), was chosen so that it would resonate with an orbit inside the separatrix. (The frequency varies with amplitude from the O-point from a maximum \( \Omega = 1 \) at the O-point to \( \Omega = 0 \) at the separatrix.) The dots in figure 3 show the Poincaré surface of section for a time-\( T \)-map, with \( T = 2\pi/\omega \). The elliptic point (O-point) of a resonant \( m = 1 \) island is clearly seen near \((q, p) = (-0.35, 0)\). We see that indeed the time dependent step size variations lead to an unphysical parametric resonance for the Hamiltonian system in equation (18).

3. Integration with variable time step \( \Delta(q, p) \)

We now turn from considering the time step variation \( \Delta(t) \) to variations of the form \( \Delta(q, p) \). This form of variation is perhaps more natural, since it arises when trying to optimize the time step to reduce errors in the integration method applied to an autonomous system. (We will return to this issue in section 4.) In this section, we first discuss the problems that arise with this variation, and then we describe two methods by which these problems can be resolved.

Previous attempts to apply this type of time step variation to symplectic integrators have suffered from one main, although sometimes unrecognized, problem: the equations are no longer Hamiltonian. As has been pointed out [12, 13], integration of Hamiltonian’s equations

\[
\frac{dz_i}{dt} = \epsilon_{ij} \frac{\partial H(z, t)}{\partial z_j}, \tag{19}
\]

with variable time steps satisfying \( \rho(q, p) dt = d\tau \) is equivalent to changing the time variable \( t \) to \( \tau \), and integrating the following equations with fixed size steps in \( \tau \); \( \Delta \tau = h \):

\[
\frac{dz_i}{d\tau} = \frac{1}{\rho(z)} \epsilon_{ij} \frac{\partial H(z, \tau)}{\partial z_j}, \frac{d\tau}{dt} = \frac{1}{\rho(z)}, \tag{20}
\]

where \( \epsilon_{12} = -\epsilon_{21} = 1, \ \epsilon_{11} = \epsilon_{22} = 0 \) (summation assumed). Here, \( z = (q, p) \). As they stand, these equations are not in canonical Hamiltonian form. Because of this, application of an integrator which is symplectic for a Hamiltonian system should not be expected to give results that are symplectic, since equations (20) do not represent a canonical Hamiltonian flow.

Once this problem has been identified, there are various approaches that can be used to find an integrator which preserves the Hamiltonian nature of equation (19), even with time steps given by \( \rho(q, p) dt = d\tau \). In the rest of this section, we review and discuss two methods for integrating equations (20) in such a way that the symplectic nature of the original equations (equation (19)) is preserved. The first method is to embed these equations into a larger phase space, considering \( t \) to be another coordinate. This extended phase space approach goes back to the work of Sundman [27], and has more recently been applied to numerical methods, both non-symplectic [28] and symplectic [12, 13]. In the extended phase space, the new equations can again be written in canonical Hamiltonian form, and thus integrated with any (fixed \( \tau \) step) symplectic integrator. This extended phase space method is not the only way to integrate equations (20) symplectically, however. A second method which we consider in this section (which only applies to one degree of freedom problems) is to recognize the the equations can be written in terms of a non-canonical bracket. Any method which preserves this bracket will then have all the nice properties of a symplectic integrator for a canonical system. We present a novel generating function approach for constructing such a method.

For the numerical results presented in this section, we will consider the Hamiltonian with a cubic potential given in equation (18), integrated by the two different methods. The variable time steps \( \Delta = \Delta(q, p) \) are chosen so they might appear to have an \( m = 1 \) resonance, since that is what is expected to give islands similar to the previous results of figure 3. Let

\[
\Delta(q, p) = \Delta_0 (1 + a_1 q + a_2 p). \tag{21}
\]

For the simulations reported in this paper, \( a_1 = 0.5 \) and \( a_2 = 0.25 \).\(^4\) For \( \rho(q, p) \Delta(q, p) = h \), i.e. \( \Delta t = \Delta(q, p) \) and \( \Delta \tau = h \), we have

\[
\rho(q, p) = \frac{h}{\Delta(q, p)} = \frac{h}{\Delta_0 (1 + a_1 q + a_2 p)}. \tag{22}
\]

The step size \( \Delta \tau = h \) was held fixed, and \( \Delta_0 \) was adjusted so that after a given number \( N \) periods of the orbit, \( t(N) \) equals \( \tau(N) \). This is done so that the differences between the original and extended phase space results are due to the

\(^4\) We take \( a_2 \neq 0 \) in order to make the equations asymmetric in \( p \). Otherwise, the symmetry of CN makes the results appear symplectic, when in general they would not be.
step size variation, rather than a change in the average step size. Integrating the original Hamilton equations (19) with fixed step size CN (i.e., with \( a_1 = a_2 = 0 \)) gives a result with bounded errors in energy (see figure 4), as is expected for symplectic integrators. However, integrating equations (19) using CN with step size given by equation (22) gives errors in energy with linear growth, as also seen in figure 4. This lack of boundedness of the energy is to be expected, since varying the step size in this way is equivalent to integrating equations (20) with fixed step size, and (20) is not a Hamiltonian system. Thus there is no reason that using a symplectic method such as CN would give results with bounded errors in energy. (Note that the Hamiltonian is just a useful diagnostic; the underlying problem is that phase space area is not conserved.)

3.1. Extended phase space method

By a well-known procedure [12, 13, 27, 28], we introduce \( \rho = \rho(q, p, q_0, p_0) \) and consider the Hamiltonian in extended phase space:

\[
K(q, p, q_0, p_0) = \frac{1}{\rho(z)} \left( H(q, p, q_0) + p_0 \right),
\]

again with \( z = (q, p) \). The canonical equations of motion are

\[
\frac{dq}{d\tau} = \frac{1}{\rho(z)} \frac{\partial H(q, p, q_0)}{\partial p} + (H + p_0) \frac{\partial}{\partial p} \left( \frac{1}{\rho} \right),
\]

\[
\frac{dp}{d\tau} = -\frac{1}{\rho(z)} \frac{\partial H(q, p, q_0)}{\partial q} - (H + p_0) \frac{\partial}{\partial q} \left( \frac{1}{\rho} \right),
\]

\[
\frac{dq_0}{d\tau} = \frac{\partial K}{\partial p_0} = \frac{1}{\rho(z)},
\]

\[
\frac{dp_0}{d\tau} = -1 \frac{\partial K}{\partial q_0} = -\frac{1}{\rho(z)} \frac{\partial H}{\partial q_0}.
\]

The last of these equations implies that if we choose \( p_0(\tau = 0) = -H(q(0), p(0), 0) \), then \( dp_0/d\tau = -dH/d\tau \) and \( H + p_0 \) remains zero. In this case, equations (24) are identical to equations (20). So, with this choice of initial condition for \( p_0 \), the actual orbit is followed and \( K = 0 \). Note that, for this value of \( p_0 \), the other contours of \( K = \) const. are not orbits of the original system.

With the equations of motion in the form (24), we can then use a canonical symplectic integrator such as modified LF (ML) (a semi-implicit, symmetrized version of LF; see [29, 30]) or CN, both with fixed time step \( \Delta \tau = h \). This is the method used in [12, 13] to integrate Hamiltonian equations of motion with variable time steps for the special case \( \partial H/\partial t = 0 \), for which \( H \) and \( p_0 \) are separately constants of motion. It should be noted that in a symplectic integration of equations (24), \( H + p_0 \) will be only approximately invariant, so that the results of numerically integrating equations (24) will have small errors relative to the numerical results of integrating equations (20).

Note that if \( H \) is independent of \( t \), then one needs only to integrate the equations for \( q \) and \( p \), since \( p_0 \) is exactly constant, and \( q_0 = t \) can be found by post-processing. So, even though this method ‘extends’ phase space, the dimension of the system effectively remains unchanged. Therefore, we do not expect parametric instability.

3.2. Numerical results: extended phase space method

In this section we report numerical results using the extended phase space method (equation (24)) to integrate the equations from the cubic Hamiltonian (equation (18)), using \( \rho(q, p) \) as given in equation (22). In figure 5 the energy errors are compared for (a) CN integration and (b) ML integration. In both cases, the black curve gives the extended phase space results, while the gray curve gives the result obtained by applying the same method with fixed step size to the original Hamiltonian equations. As for figure 4, the \( \tau \) step \( h \) was chosen to make \( \tau(N) \) equal to \( t(N) \) after \( N \) periods of the orbit. We conclude that there is no secular change in the value of the Hamiltonian \( H(q(t), p(t)) \). The time step in equation (22) was chosen because it appears at first to have potential for an \( m = 1 \) resonance, not in order to reduce errors; in section 4 we will describe a method to minimize the integration errors.

A surface of section plot for the extended phase space CN integration is shown in figure 6. In contrast to figure 3, there is no resonant island caused by the time step variation. This is consistent with the comment at the end of section 3.1.

As a final check of the extended phase space method, a comparison was made between integrating equations (20) where the step size is determined by the position in phase space as \( \Delta(q, p) \propto 1/\rho(q, p) \), and integrating equation (19) where the step size is a function of time as determined by a reference orbit \( \Delta(t) \propto 1/\rho(q_{ref}(t), p_{ref}(t)) \). The reference orbit was obtained by solving the extended phase space equations (equations (20)), for some initial conditions \((q_0, p_0)\) for which the period is \( T(q_0, p_0) \). Time-\( T \) surface of section plots for several cases give results qualitatively similar to figure 3, with the time dependent step size \( \Delta(t) = \Delta(q_{ref}(t), p_{ref}(t)) \) giving a resonant island centered at the location of the reference orbit.

That is, \( \Delta(t) \) is unstable when \( \Delta(q, p) \) is stable, even when the time steps are equal on the reference orbit. This behavior is similar to the secular and unstable cases of perturbation theories discussed in appendix A.

3.3. Non-canonical symmetrized leapfrog

In this section we discuss a second method used to integrate equations (20), which works for one degree of freedom systems...
This measure preservation suggests that a measure preserving integrator applied to this system would have the same nice properties of a symplectic integrator applied to a canonical Hamiltonian system.

The equations of motion in the form in equations (20) are not canonical Hamiltonian equations. However, in one degree of freedom, equations (20) are a Hamiltonian system in non-canonical variables and can be written in the form

$$\frac{\dd z_i}{\dd \tau} = [z_i, H]_c, \quad \text{where } [f, g] = \frac{1}{\rho(z)} \frac{\partial f}{\partial z_j} \frac{\partial g}{\partial z_i}$$

(26)

is a non-canonical bracket. That is, it is antisymmetric, and direct calculation shows that it satisfies the Jacobi identity $$[f, [g, h]], + [g, [h, f]], + [h, [f, g]]] = 0.$$ A method of constructing a symplectic non-canonical integrator in terms of generating functions [31] starts with the condition that must hold for the time-$$t$$ map, which is that it must preserve the two-form

$$\rho(x, y) \, dx \wedge dy = \rho(X, Y) \, dX \wedge dY,$$

(27)

See appendix B for more details regarding this condition. First, we define

$$\eta(x, y) = \int^y \rho(x, y') \, dy'$$

(28)

and

$$\xi(x, y) = \int^x \rho(x', y) \, dx'.$$

(29)

With these definitions, we can write

$$\rho(x, y) \, dx \wedge dy = dx \wedge d\eta(x, y),$$

(30)

$$\rho(X, Y) \, dX \wedge dY = d\xi(X, Y) \wedge dY$$

(31)

and therefore equation (27) becomes

$$dx \wedge d\eta(x, y) = d\xi(X, Y) \wedge dY.$$ 

(32)

We can consider $$(X, Y)$$ to be functions of $$(x, y),$$ and then define $$p = \eta(x, y)$$ and $$Q = \xi(x, Y).$$ These definitions, together with equation (32), imply that the one-form

$$\omega = p \, dx + Q \, dY$$

(33)

is exact, i.e. $$d\omega = 0.$$ This in turn implies

$$\omega = dF(x, Y) = \frac{\partial F(x, Y)}{\partial x} \, dx + \frac{\partial F(x, Y)}{\partial Y} \, dY,$$

(34)

at least locally. We are led to the relations

$$\eta(x, y) = p = \frac{\partial F(x, Y)}{\partial x},$$

(35)

$$\xi(X, Y) = Q = \frac{\partial F(x, Y)}{\partial Y}.$$ 

(36)

Given the generating function $$F(x, Y),$$ we solve equation (35) for $$Y(x, y)$$ and then substitute into equation (36) to obtain $$X(x, y).$$

In essence, what is going on is this: we are transforming to canonical variables $$(x, p)$$ and $$(Q, Y),$$ where $$p = \eta(x, y)$$ and $$Q = \xi(X, Y).$$ Then we are performing a canonical
transformation \((x, p) \rightarrow (Q, Y)\) in terms of a generating function \(F(x, Y)\), with \(Q = \partial F/\partial Y\) and \(p = \partial F/\partial x\), and expressing the results in terms of \((x, y)\), and \((X, Y)\).

The identity transformation has \(X = x\) and \(Y = y\) so that equations (35), (36) take the form
\[
\eta(x, y) = \frac{\partial F_0(x, y)}{\partial x}, \quad (37)
\]
\[
\xi(x, y) = \frac{\partial F_0(x, y)}{\partial y}. \quad (38)
\]

These relations ensure that \(\partial \eta(x, y)/\partial y = \partial \xi(x, y)/\partial x = \partial^2 F_0/\partial x \partial y\); by equations (28) and (29), these both equal \(\rho(x, y)\), which is non-zero. This nondegeneracy is necessary for the inversions in equations (35) and (36) to work.

We now wish to construct an \(O(h)\) approximation to \(F(x, Y)\) in order to find a time-\(h\) map \((h = \Delta \tau)\) for the system given by equations (20). Let us try the generating function
\[
F(x, Y) = F_0(x, y) + hH(x, y). \quad (39)
\]

From equations (35) and (36) we find
\[
\eta(x, y) = \frac{\partial F_0}{\partial x} - hv(x, y), \quad (40)
\]
\[
\xi(X, Y) = \frac{\partial F_0}{\partial Y} + hu(x, y), \quad (41)
\]
where \(u(x, y) = \partial H(x, y)/\partial y\) and \(v(x, y) = -\partial H(x, y)/\partial x\).

Substituting equations (37) and (38) into these equations gives
\[
\eta(x, y) = \eta(x, y) - hv(x, y), \quad (42)
\]
\[
\xi(X, Y) = \xi(x, y) + hu(x, y). \quad (42)
\]

This is the form of our integrator: we integrate \(\rho\) to give \(\eta(x, y)\) and \(\xi(x, y)\) as in equations (28) and (29), iterate the first of (42) to solve for \(Y\) and, after substituting for \(Y\), iterate the second of (42) to solve for \(X\). We do not need the explicit form for \(F_0\) or the Hamiltonian \(H\).

In order to see that equations (42) are a first order accurate integrator for the system in equations (20), we expand to first order in \(h\), and find
\[
0 = (Y - y)\frac{\partial \eta(x, y)}{\partial y} - hv(x, y) + O(h^2) \quad (43)
\]
\[
(X - x)\frac{\partial \xi(x, y)}{\partial x} = hu(x, y) + O(h^2). \quad (44)
\]

With equations (28), (29), this leads to
\[
X = x + h\frac{u(x, y)}{\rho(x, y)} + O(h^2), \quad Y = y + h\frac{v(x, y)}{\rho(x, y)} + O(h^2). \quad (45)
\]

This implies that equations (42) do constitute a first order accurate integrator for equations (20). It is clear that the scheme in equations (42) is the non-canonical form of the ML integrator [29, 30]. Note, however, that the system in equations (42) is implicit in both \(X\) and \(Y\).

For the complementary generating function \(G(X, y)\) we follow the same procedure, defining \(\xi(x, y)\) and \(\eta(x, y)\) exactly as in equations (28) and (29). We can now write equation (27) as
\[
d\xi(x, y) \wedge dy = dX \wedge d\eta(X, Y), \quad (46)
\]
which, together with the definitions \(P = \eta(X, Y)\) and \(q = \xi(x, y)\), implies that
\[
\omega' = -q dy - P dx \quad (47)
\]
is exact \((\omega' = 0)\). Therefore \(\omega' = dG(X, y) = (\partial G(X, y)/\partial x) dx + (\partial G(X, y)/\partial y) dy\) and
\[
\xi(x, y) = -\frac{\partial G(X, y)}{\partial y}, \quad (48)
\]
\[
\eta(X, Y) = -\frac{\partial G(X, y)}{\partial x}. \quad (49)
\]
The identity is given by \(G_0(X, y)\), where
\[
\xi(x, y) = -\frac{\partial G_0(x, y)}{\partial y}, \quad (50)
\]
\[
\eta(X, Y) = -\frac{\partial G_0(x, y)}{\partial x}, \quad (50)
\]
with \(-\partial^2 G_0/\partial x \partial y = \rho(x, y)\). We try \(G(X, y) = G_0(X, y) + hH(X, y)\), which leads to
\[
\xi(x, y) = \xi(x, y) - hu(x, y), \quad (50)
\]
\[
\eta(X, Y) = \eta(x, y) + hv(x, y). \quad (50)
\]
As in the case with equations (42), this is the form we use as an integration scheme, and it is not necessary to obtain \(G_0\) explicitly. Finally, a first order expansion in \(h\) again gives equations (45), showing that equations (50) are also a first order accurate integrator for equations (20).

The first order maps \((x, y) \rightarrow (X, Y)\) defined by equations (42) and equations (50) involve integration of a one degree of freedom Hamiltonian system with no explicit time dependence, and thus do not exhibit a parametric instability for small enough time steps.

We have shown that both schemes in equation (42) and in equation (50) are first order accurate integrators for equations (20). What remains is to show that if they are applied sequentially one obtains second order accuracy. The first point is that if the maps based on \(F(x, Y)\) and \(G(X, y)\) are written as \(T_F(h)\) and \(T_G(h)\), respectively, one can show that
\[
T_F^{-1}(h) = T_G(-h) \quad (51)
\]
and of course \(T_G^{-1}(h) = T_F(-h)\). This follows from inspection of equations (42) and (50).

The composed map is \(T(h) = T_G(h/2) \circ T_F(h/2)\) and we find
\[
T^{-1}(h) = T_F(h/2)^{-1} \circ T_G(h/2)^{-1} = T_G(-h/2) \circ T_F(-h/2) = T(-h). \quad (52)
\]
Thus, \(T(h)\) is time symmetric and is therefore second order accurate\(^6\). We call \(T(h) = T_G(h/2) \circ T_F(h/2)\) non-canonical symmetrized leapfrog (NSL).

The methods outlined in this section preserve the non-canonical bracket, as does the actual time evolution of the
non-canonical system. Integrators with this property are often called Poisson integrators [19–22].

It is interesting to note in this context that (fixed step size) CN can be written as \( T_{CN}(h) = T_f(h/2) \circ T_b(h/2) \), where \( T_f \) is forward (explicit) Euler and \( T_b \) is backward (implicit) Euler. Further, the implicit midpoint method \( x' = x + (h/2)u(x) + (h/2)u(x') \) can be written as \( T_{mid}(h) = T_f(h/2) \circ T_b(h/2) \). This shows that \( T_{mid} = T_f(h/2)^{-1} \circ T_{CN}(h) \circ T_f(h/2) \), so that the implicit midpoint method is related to CN by a non-canonical change of variables. This implies that the implicit midpoint method is equivalent to a symplectic method under a (non-symplectic) change of variables, so it is a Poisson integrator. Therefore it can be used to integrate a canonical Hamiltonian system with all the advantages of a symplectic integrator.

3.4. Numerical results: non-canonical symmetrized leapfrog

In this section we report numerical results where the non-canonical symmetrized leapfrog (NSL) integration scheme is applied to the cubic Hamiltonian (equation (18)), with \( \rho(x, y) = h^2/\Delta_1^2(1 + a_1x + a_2y) \), as given in equation (22). Integrating \( \rho(x, y) \) yields \( \eta(x, y) = h \ln(1 + a_1x + a_2y)/\Delta_1 \) and \( \xi(x, y) = h \ln(1 + a_1x + a_2y)/\Delta_0 \), and thus equation (42) with this Hamiltonian and time step variation becomes

\[
\begin{align*}
\eta(x, y) &= \ln(1 + a_1x + a_2y)/\Delta_1, \\
\xi(x, y) &= \ln(1 + a_1x + a_2y)/\Delta_0.
\end{align*}
\]

This implies that the implicit midpoint method is related to CN by a non-canonical change of variables. This implies that the implicit midpoint method is equivalent to a symplectic method under a (non-symplectic) change of variables, so it is a Poisson integrator. Therefore it can be used to integrate a canonical Hamiltonian system with all the advantages of a symplectic integrator.

4. Using error estimates to find \( \Delta(q, p) \)

We next turn our attention to the choice of step size variation \( \Delta = \Delta(q, p) \), based on an error estimator. Basing the choice of \( \Delta \) on an error estimate will give step size variations which are optimized to reduce errors, in a manner to be defined.

Figure 7. The NSL method applied to the cubic oscillator, with time step variations as given in equation (22). Shown in black is the error in energy. For comparison, in gray is shown the error in energy for fixed step size symmetrized LF. Parameters: \( h_0 = 0.05 \), \( \Delta_0 = 1.0524 \), \( (q_0, p_0) = (0.3, 0) \), \( a_1 = 0.5 \), \( a_2 = 0.25 \).

4.1. Error estimates and minimization

As an example of an error estimate we consider CN integration of \( dz/dt = u(z) \), where again \( z = (x, y) \). Namely, we define a map \( z' = T_b(z) \) given by

\[
z' = z + \Delta u \left( \left[ (z + z')/2 \right] \right),
\]

where \( z = z(t) \) and \( z' = z(t + \Delta t) \), where \( \Delta = \Delta t \) can vary as a function of \( z \). If \( u \) comes from a Hamiltonian system, CN is symplectic, but that property is not important for these considerations. We can thus let \( \Delta(t) = \Delta(q_{ref}(t), p_{ref}(t)) \), where \( q_{ref} \) and \( p_{ref} \) are the exact orbits\(^\text{7} \). As mentioned in section 2.1, there will be terms proportional to \( d\Delta/dt \), but they will appear at the next order in \( \Delta \).

The error estimate is found by expanding \( z(t + \Delta t) \) in \( \Delta \), and performing backward error analysis to obtain a local error estimate. This is a very different objective than that in the backward error analysis in section 2. In index notation we obtain

\[
\frac{d\tilde{z}_i}{dt} + \frac{\Delta}{2} \frac{d^2 \tilde{z}_i}{dr^2} + \frac{\Delta^2}{6} \frac{d^3 \tilde{z}_i}{dr^3} = u_i \left( \frac{z + \Delta}{2} \right) + \frac{\Delta^2}{4} \frac{d^2 z}{dr^2} = u_i(z) + \frac{\Delta}{2} \frac{\partial z}{\partial u_i} \frac{\partial u}{\partial z} + \frac{\Delta^2}{8} \frac{\partial^2 z}{\partial u_i \partial u_j} \frac{\partial u_j}{\partial z}.
\]

This leads to

\[
\frac{d\tilde{z}_i}{dt} = \tilde{u}_i + \frac{\Delta}{2} \left( \frac{1}{12} u_k u_j u_{i,j} - \frac{1}{24} u_{i,k} u_{i,j} \right),
\]

which can be written in vector notation as

\[
\frac{dz}{dt} = u + \frac{\Delta}{2} \left( \frac{1}{12} (u \cdot \nabla u) \cdot \nabla u - \frac{1}{24} u \cdot (\nabla \nabla u) \cdot u \right),
\]

where \( u = u(z(t)) \).

\(^7\) Also, since we are considering \( \Delta = \Delta(t) \), we do not need the terms proportional to \( H + p_0 \) in the extended phase space method, equation (24). Regardless of the form of \( \Delta \), this term is of higher order than the error we are estimating in this calculation.
Writing the error per time step as \( e = \Delta^2 w(t) \), where \( w(t) = [(u \cdot \nabla u) \cdot \nabla u]_{12} - u \cdot (\nabla \nabla u) \cdot u/24] \), the total error in an integration is

\[
E = \int_0^T e \, dt = \int_0^T \Delta^2 w(t) \, dt. \tag{59}
\]

Now if we write the variable time step \( \Delta t \) as \( \Delta t = (dt/d\tau) h \), where \( h = \Delta \tau \) is the constant step size in \( \tau \), this error takes the form

\[
E = h^2 \int \, dt \left( \frac{dt}{\Delta \tau} \right)^3 w(t). \tag{60}
\]

We proceed to minimize the total error \( E \) by writing

\[
E = h^2 \int \, dt \left( \frac{dt}{\Delta \tau} \right)^3 w(t).
\]

\[
\text{We obtain } H = 2(\beta/3)^{3/2} w(t)^{-1/2}. \text{ Notice that the Hamiltonian } H \text{ is independent of the time } \tau \text{ and is therefore a constant of motion. Also, the Hamiltonian } H \text{ is proportional to the Lagrangian } L = (\partial q/\partial \tau, \partial p/\partial \tau) \text{ as a function of } \tau \text{ and } H = \beta w(t)^{3/2} \text{, implying that } L \text{ is also a constant. Since } \partial q/\partial \tau = 1/\rho, \text{ we obtain an expression for the optimized time steps:}
\]

\[
\rho_{opt}(z(t)) = C w(t)^{1/3}. \tag{64}
\]

This condition says that the Lagrangian, the integrand in equation (60), is constant with respect to \( \tau \). (But the local error \( e \) in equation (59) is not constant with respect to \( t \).) A condition of this form is called an equidistribution principle [32].

### 4.2. Numerical results

In order to test the optimized time step, we compare numerical results using constant time step \( \Delta = \Delta_0 \), the optimized time step

\[
\Delta_{opt} = C_{opt} w(q, p)^{1/3} \propto 1/\rho_{opt}, \tag{65}
\]

and time steps designed to give equal arc length:

\[
\Delta_{arc} = C_{arc} \left[ \left( \frac{\partial H}{\partial p} \right)^2 + \left( \frac{\partial H}{\partial q} \right)^2 \right]^{-1/2}. \tag{66}
\]

With \( \Delta_{arc} \), the magnitude of the phase space velocity \( \bar{v} = (\partial q/\partial \tau, \partial p/\partial \tau) \) is constant. Numerical results for these three choices of \( \Delta \) are shown in figure 8, using the CN integrator in extended phase space. For each of these methods, fixed steps in \( \tau \) of size \( \Delta \tau = h \) were used. The constant of proportionality \( C \) in \( \Delta = C/\rho \) was then chosen so that, after \( N \) periods of the orbit, \( \tau(N) \) equals \( t(N) \). This is done in order to distinguish

\[
\text{the effect of varying the step size as a function of } (q, p) \text{ from the effect of reducing the overall average step size.}
\]

Two diagnostics of the numerical integrations related to the local error are shown in figure 8, for \( \Delta = \Delta_0 \) (light gray), \( \Delta_{arc} \) (dark gray) and \( \Delta_{opt} \) (black). (a) The local error as a function of time \( t \) (integrand of equation (59)), and (b) the local error as a function of \( \tau \) \( (h^3 \text{ times the integrand of equation (60)}) \). Parameters: \( h = 0.1, (q_0, p_0) = (0.4, 0), \Delta_0 = 0.1, C_{arc} = 0.41, C_{opt} = 0.28 \)

\[
\text{for comparison, using } \Delta = \Delta_{opt} \text{ gives } E = 2.48 \times 10^{-4}, \text{ and } \Delta = \Delta_0 \text{ const. gives } E = 3.29 \times 10^{-4}
\]

### 5. Summary

In this paper, we have studied variable and adaptive time stepping for symplectic integrators, of importance for particle-in-cell codes, for accelerators, for tracing magnetic field lines,
and for ray tracing. We have shown that problems observed in the literature for symplectic integrators with variable time steps fall into two categories. In the first, with time step variation $\Delta = \Delta(t)$, the integrators are still symplectic but results can exhibit parametric instabilities associated with resonances between the time step variation and the orbital motion. We have characterized these instabilities by means of backward error analysis and numerical integrations. In the second category, the time steps depend on position in phase space, $\Delta = \Delta(q,p)$, and integrators which are symplectic for $\Delta = \text{const.}$ are no longer symplectic.

We have discussed symplectic integrators for $\Delta = \Delta(q,p)$ of two basic varieties. In both, we start by modifying the time variable $t \rightarrow \tau$ such that $\rho(q,p) dt = d\tau$ and $\rho(q,p) \propto \Delta(q,p)^{-1}$ and we do uniform time stepping in $\tau$. In the first method, one extends the phase space $(q_1, \ldots, q_n, p_1, \ldots, p_n) \rightarrow (q_0_q, q_1, \ldots, q_n, p_0, p_1, \ldots, p_n)$, with $q_0 = t$ and $p_0$ its canonical conjugate. In this extended phase space with $\tau$ taking the place of time and $\Delta \tau = \text{const.}$, any numerical integrator can be used and we investigate modified leapfrog methods

$$\text{secularities show up in perturbation theories in the following manner. Take the system}$$

$$\ddot{x} + x + \epsilon x^3 = 0. \quad (A.1)$$

A straightforward perturbation method involves iterating

$$\dot{x}_{k+1} + x_{k+1} = -\epsilon x_k^3. \quad (A.2)$$

For $x_0 = b \cos t$, we obtain

$$\dot{x}_1 + x_1 = -\epsilon b^3 \left( \frac{1}{2} \cos 3t + \frac{3}{2} \cos t \right). \quad (A.3)$$

Two main time step variations are considered in the literature:

$\Delta = \Delta(t)$ and $\Delta = \Delta(q,p)$. The phase space dependent variation $\Delta(q,p)$ is natural because the errors in an integration method of an autonomous system depend only on phase space position. Indeed, we found that error analysis (as in section 4) for the integration method gives errors which depend on location in phase space $(q,p)$.

The second kind of variation $\Delta(t)$ comes from a type of perturbation analysis. The logic is as follows: orbits $(q(t), p(t))$ of a Hamiltonian system are often periodic, and because of this, time step variations $\Delta(q,p)$ on the orbit should also be periodic. That is, we can substitute $q(t)$ and $p(t)$ to arrive at $\Delta(t) \equiv \Delta(q(t), p(t))$, giving periodic time dependence.

This argument ignores the stability issue: if an orbit is perturbed, the period of $\Delta(q(t), p(t))$ will vary, but this will not occur for $\Delta(t)$ prescribed from the unperturbed orbit.

It has been observed [6, 8–10] that such a $\Delta(t)$ is not a stable method for varying the time step of a symplectic integrator. Some analysis (see [17] and section 2) shows that this does not work because it introduces parametric resonances into the system. As we have shown in section 2, the integrator is still symplectic in this case, but the problem is that the modified equations (in the case of a harmonic oscillator) take the form of the Mathieu equation, which is still Hamiltonian but can be unstable.

We here review how such parametric instabilities and secularities arise in perturbation theory, to help us understand the parametric instabilities of section 2.1.

Secularities show up in perturbation theories in the following manner. Take the system

The model Hamiltonian system and found that indeed the error is minimized while the advantages of symplectic integration are preserved.

Acknowledgments

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Appendix A. Variable time steps and perturbation methods

Figure 9. The global error (equation (60)), over the time $T = 20$, for the time step variation $\Delta t$ (equation (67)). As seen in the inset, the error is minimized with $E = 2.22 \times 10^{-4}$ for $\beta = 1$, for which $\Delta t = \Delta t_{\text{opt}}$. For comparison, using $\Delta t = \Delta t_{\text{const}}$ gives $E = 2.48 \times 10^{-4}$, and $\Delta t = 0$ gives $E = 3.29 \times 10^{-4}$.
The last term on the right is resonant and leads to a secularity,
\[ x_1 = b \cos t - \frac{3eb^3}{8} t \sin t + \cdots. \] (A.4)

However, it is clear from equation (A.1) that the exact solution is bounded: the energy is \( H = \dot{x}^2/2 + x^2/2 + \epsilon x^4/4 \).

The term \( \dot{t} \sin t \) represents the frequency shift that occurs in equation (A.1) because of the term proportional to \( \epsilon \), and is accurate for short time, but clearly wrong for long time.

For an example of a perturbation approach with a parametric instability, we consider instead
\[ \ddot{x} + x + \epsilon x^2 = 0, \] (A.5)
with the perturbation method
\[ \ddot{x}_{k+1} + x_{k+1} = -\epsilon x_k x_{k+1}. \] (A.6)

(We choose a different model in order to obtain again results at first order in the perturbation theory.) From \( x_0 = b \cos t \) we obtain
\[ \dot{x}_1 + (1 + \epsilon b \cos t) x_1 = 0. \] (A.7)

Using \( t = \tau/2 \), this is the Mathieu equation \( d^2x/d\tau^2 + (a + 2\epsilon b \cos 2\tau)x_1 = 0 \), with \( a = 4 \) and \( q = 2\epsilon b \), for which a parametric instability occurs. As in the secular example above, the exponential growth represents the correct frequency shift for small time, but is wrong for longer time. Indeed, the energy is \( H = \dot{x}^2/2 + x^2/2 + \epsilon \dot{x}^4/3 \), and for initial conditions near \( \dot{x} = 0 \) the solution cannot grow indefinitely. As we have seen in section 3.1, parametric instabilities for \( \Delta t = \Delta (\tau) \) have a very similar character.

**Appendix B. Non-canonical brackets and forms**

In this appendix we first describe the conditions that change of variables must satisfy so that the form of a set of equations defined with a non-canonical bracket is preserved. We then show that the flow of a Hamiltonian system written in non-canonical variables, such as equations (20) (one degree of freedom), generates a change of variables satisfying these conditions.

First define the non-canonical bracket
\[ [f(z), g(z)]_\epsilon \equiv \frac{1}{\rho(z)} \epsilon_{ij} \frac{\partial f(z)}{\partial z_i} \frac{\partial g(z)}{\partial z_j}. \] (B.1)

In one degree of freedom, \([\cdot, \cdot]_\epsilon \) is indeed a non-canonical bracket, which can be verified by proving the Jacobi identity. In more than one degree of freedom, this does not define a legitimate non-canonical bracket, since it does not satisfy the Jacobi identity.

We now ask what change of variables \( Z = Z(z) \) preserves the form, i.e. what conditions must this change of variables satisfy so that
\[ [f(z), g(z)]_\epsilon = [f(Z), g(Z)]_\epsilon, \] (B.2)
where
\[ [f(Z), g(Z)]_\epsilon \equiv \frac{1}{\rho(Z)} \epsilon_{mn} \frac{\partial f(Z)}{\partial Z_m} \frac{\partial g(Z)}{\partial Z_n}. \] (B.3)

Using the definitions of these brackets and the chain rule, equation (B.2) becomes
\[ \frac{1}{\rho(z)} \epsilon_{ij} \frac{\partial Z_m}{\partial z_i} \frac{\partial f(Z)}{\partial Z_m} \frac{\partial g(Z)}{\partial Z_n} = \frac{1}{\rho(Z)} \epsilon_{mn} \frac{\partial f(Z)}{\partial Z_m} \frac{\partial g(Z)}{\partial Z_n}. \] (B.4)

In order for this to be true, we require that
\[ \frac{1}{\rho(z)} \epsilon_{ij} \frac{\partial Z_m}{\partial z_i} \frac{\partial Z_n}{\partial z_j} = \frac{1}{\rho(Z)} \epsilon_{mn}, \] (B.5)
or, written in matrix form, that
\[ \text{MEM} = \frac{\rho(z)}{\rho(Z)} E, \] (B.6)
where \( M_{ij} = \frac{\partial Z_i}{\partial z_j}, \ E_{ij} = \epsilon_{ij}. \)

If this condition is satisfied, then the transformation \( z \to Z \) preserves this specific non-canonical symplectic structure.

The next issue is to show that the time evolution operator for equations (20) generates a map with this property. Since equations (20) can be written in terms of the non-canonical bracket as
\[ \frac{dz_i}{d\tau} = [z_i, H]_\epsilon, \] (B.7)
then, for infinitesimal \( \delta \), if we define \( z_i = z_i(0) \) and \( z_i = z_i(\delta) \) we have
\[ z_i = z_i + h[z_i, H]_\epsilon. \] (B.8)

Taking the bracket of \( Z_i \) and \( Z_j \), therefore gives
\[ [Z_i, Z_j]_\epsilon = [z_i, z_j]_\epsilon + h[[z_i, H]_\epsilon, z_j]_\epsilon + h[z_i, [z_j, H]_\epsilon]_\epsilon \]
\[ = [z_i, z_j]_\epsilon + h[[z_i, H]_\epsilon, z_j]_\epsilon + h[H, [z_j, H]_\epsilon]_\epsilon \]
\[ = [z_i, z_j]_\epsilon + h[[z_i, H]_\epsilon, z_j]_\epsilon. \] (B.9)

The last equality follows from the Jacobi identity. This equals
\[ [Z_i, Z_j]_\epsilon = \epsilon_{ij} \left( \frac{1}{\rho(z)} h[1/\rho, H] \right) \]
\[ = \epsilon_{ij} \left( \frac{1}{\rho(z)} + (Z_k - z_k) \frac{\partial}{\partial z_k} \left( \frac{1}{\rho(z)} \right) \right) \]
\[ = \epsilon_{ij} \frac{\rho(Z)}{\rho(Z)} = [Z_i, Z_j]_\epsilon. \] (B.10)

Thus, the time evolution operator for an infinitesimal time step \( \delta \) preserves the non-canonical symplectic structure. This fact is the basis for finding a non-canonical generating function in section 3.3 that gives a first order accurate integrator for the non-canonical Hamiltonian system.

Finally, we express these ideas in terms of differential forms. Equation (B.5) can be written as
\[ \rho(Z) \frac{\partial Z_k}{\partial z_i} \epsilon_{kl} \frac{\partial Z_l}{\partial z_j} = \rho(z) \epsilon_{ij}. \] (B.15)

From this, we obtain the expression
\[ \rho(Z) \{\partial Z_k/\partial z_i\} \epsilon_{kl} (\partial Z_l/\partial z_j) dz_k dz_j = \rho(z) \epsilon_{ij} dz_i dz_j \] (B.16)
or
\[ \rho(Z) \epsilon_{kl} dz_k dZ_l = \rho(z) \epsilon_{ij} dz_i dz_j. \] (B.17)

Since we are considering only 2D phase space, this can be expressed as
\[ \rho(X, Y) dX \wedge dY = \rho(x, y) dx \wedge dy. \] (B.18)
Equation (B.18) is the two-form used in section 3.3.
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