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# Does variable step size ruin a symplectic integrator? *

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There exist methods that preserve the symplectic invariants of Hamiltonian systems when fixed step size is used. It is proved that the most simple-minded version of this property is lost if the step size is varied.

## 1. Discussion

There is currently great interest [1,2] in numerical methods that preserve symplectic invariants for Hamiltonian systems

$$y' = JH_y(y), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

where $H$ is a scalar function of generalized momenta and an equal number of generalized positions. A one-step method $y_{n+1} = F(y_n, h)$ is said to be *symplectic*, or *canonical*, if for all (sufficiently small) step sizes $h$ and all appropriate Hamiltonians $H$ we have

$$F_y^{\mathrm{T}} J F_y = J. \tag{1}$$

In particular, this condition is satisfied by the $h$-flow of a Hamiltonian system. Only one-step methods seem to have this property in all fullness.

However, if we vary the step size, we actually have

$$y_{n+1} = F(y_n, h_n),$$

where $h_n$ depends on $y_n$, $h_{n-1}$, and some accuracy parameter. (Given $y_n$ and $h_{n-1}$, it is normally possible with a symplectic method to reverse the step, so there is no separate dependence on either $y_{n-1}$ nor the intermediate stage values.) Typically, the accuracy parameter would be a local error tolerance ltol. However, we use here the more familiar symbol $h$ as the accuracy parameter where $h$ is related to ltol by some simple formula. For error per step this could be $h = \mathrm{ltol}^{1/(p+1)}$ where $p$ is the order of the method. If the step size $h_n$ really does depend on $h_{n-1}$, this almost certainly increases (by one) the dimension of the phase space of the dynamics and it is very unlikely to produce a symplectic map. Let us assume that $h_n$ is independent of $h_{n-1}$. Such would be true if the step size were determined from derivatives of the Hamiltonian at the current value of time $t_n$. Moreover, this is approximately true in other situations where the step size is chosen to get the (absolute and/or relative) local error to approximate some fixed safety factor times the local error tolerance. If this were satisfied exactly, it would be an implicit equation relating $h_n$ to $y_n$ and $h$. Therefore, we assume that

$$h_n = h\theta(y_n; h),$$

where $\theta(y; 0) > 0$.

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The most simple-minded version of being symplectic is to require that the mapping $y_n \mapsto F(y_n, h\theta(y_n;h))$ be symplectic. If the method $F$ is symplectic for fixed step size and is at least second order accurate, the analysis in section 2 shows that for variable step size the method cannot be symplectic unless $\theta(y_n;h) = \theta(y_0;h) + O(h^2)$. For a first order method the analysis is easily modified to show that $\theta(y_n;h) = \theta(y_0;h) + O(h)$. In either case the step size must be asymptotically constant in order to maintain the property of being symplectic. This theoretical result is consistent with the experiments by Calvo and Sanz-Serna [1], which show inferior results for variable step size.

We have reservations about the appropriateness of requiring the mapping $y_n \mapsto F(y_n, h\theta(y_n;h))$ to be symplectic because it does not map to solution values at one single point in time – it is not the numerical approximation to the flow of the system. As an anonymous referee has pointed out, even if the method $F$ computed the exact flow of the system being integrated, the mapping $y_n \mapsto F(y_n, h\theta(y_n;h))$ would not be symplectic. This returns us to the question of why it is desirable for a method to be symplectic. We suggest two responses. One is that in some applications one is interested in doing statistical mechanics time averagings. Being symplectic would seem to be a practical necessity for uniform sampling of accessible phase space. The result in this paper suggests that variable step size with uniform weighting of each step would not be accurate. A second response is that the property of a method being symplectic has been shown [1] to be equivalent to the existence of a slightly different Hamiltonian for which the computed solution is the exact solution except for an exponentially small error. (Such a result is valuable if the quantities that we want to compute and the behavior we want to observe are not extremely sensitive to changes in the Hamiltonian.) For variable step size it is perhaps the existence of a nearby Hamiltonian that is important.

The result given above does not rule out the possibility of variable step size integrators being symplectic in the simple-minded sense. What it does say is that such an integrator will not be the result of varying the step size in a method that has been constructed to be symplectic for fixed step size.

## 2. Proof of result

For the method $y_{n+1} = F(y_n, h\theta(y_n;h))$ to be symplectic, eq. (1) must be satisfied with $F_y + hF_h\theta_y^{\mathrm{T}}$ substituted for $F_y$. This yields four terms on the left-hand side of (1). The first cancels with $J$ because of the assumption that the method is symplectic for fixed step size. The fourth vanishes because $J$ is skew symmetric. Hence, we are left with

$$uv^{\mathrm{T}} - vu^{\mathrm{T}} = 0,$$

where $u = F_y^{\mathrm{T}} J F_h$ and $v = \theta_y$. Premultiplying by $u^{\mathrm{T}} J$ and postmultiplying by $Jv$, we conclude $u^{\mathrm{T}} Jv = 0$, or, equivalently,

$$\theta_y^{\mathrm{T}} J F_y^{\mathrm{T}} J F_h = 0. \tag{2}$$

Under mild smoothness assumptions we have, because of second order accuracy,

$$F(y;h) = y + hJH_y + \tfrac{1}{2}h^2 JH_{yy}JH_y + h^3\Psi(y;h),$$

so

$$F_y = I + hJH_{yy} + O(h^2)$$

and

$$F_h = JH_y + hJH_{yy}JH_y + O(h^2).$$

Combining gives

$$JF_y^{\mathrm{T}} JF_h = -JH_y + O(h^2),$$

and using eq. (2) yields

$$0 = \theta_y^{\mathrm{T}} y'(t) + \mathcal{O}(h^2)$$

for an analytical solution $y(t)$. Finally, we have

$$\begin{aligned}\theta(y_n; h) &= \theta(y(t_n); h) + \mathcal{O}(h^2) \\ &= \theta(y_0; h) + \int_0^{t_n} \theta_y^{\mathrm{T}} y'(t)\,\mathrm{d}t + \mathcal{O}(h^2) \\ &= \theta(y_0; h) + \mathcal{O}(h^2).\end{aligned}$$

## References

[1] M.P. Calvo and J.M. Sanz-Serna, The development of variable-step symplectic integrators, SIAM J. Sci. Stat. Comput., in press.
[2] C.W. Gear, Physica D 60 (1992) 303, these Proceedings.