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# VARIABLE STEP SIZE DESTABILIZES THE STÖRMER/LEAPFROG/VERLET METHOD*

ROBERT D. SKEEL

*Department of Computer Science, University of Illinois at Urbana-Champaign, 1304 West Springfield Avenue, Urbana, Illinois 61801-2987, USA*

**Abstract.**

For fixed step-size $h$ the Störmer method is stable for the standard test equation $\ddot{y} = -\omega^2 y, \quad \omega > 0$, if and only if $h\omega < 2$. We show that for variable step size $h_n$ there does not exist a (positive) limit on $h\omega$ which ensures stability. Nor can we guarantee stability if, in addition, we limit the step size ratio $h_n/h_{n-1}$.

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The subject of this paper is the stability of the second order method due to Störmer [6] applied to the standard test equation

$$\ddot{y} = -\omega^2 y \tag{1}$$

where $\omega > 0$. For fixed step size $h$ the Störmer method, appropriately expressed, is stable if and only if $h\omega < 2$. We show that for variable step size $h_n$ there does not exist a (positive) limit on $h\omega$ which ensures stability. Nor can we guarantee stability if, in addition, we limit the step size ratio $h_n/h_{n-1}$ (except for the limitation of uniform step size). It seems that the result extends to any conventional explicit method for special second order ordinary differential equations

$$\ddot{y} = f(t, y).$$

Among explicit methods the Störmer method, in one of its various forms, is probably used more often in practice than all others combined. (Consider semi-discretized partial differential equations and molecular dynamics.)

This work was motivated by an investigation of symplectic methods for Hamiltonian systems, see [5] and references cited therein. Symplectic methods, such as the Störmer method, preserve certain abstract invariants of Hamiltonian systems.

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Experiments [2, 3] show that symplectic methods with uniform step size give remarkable accuracy for long integration intervals but that this does not happen with variable stepsize. We were wondering whether linearized stability theory can account for the observed behavior of symplectic methods, for it has been shown by Suris [7] that symplectic methods for special separable Hamiltonian systems are stable for sufficiently small values of $h\omega$ with uniform step size. However, numerical experiments [4] show that variable stepsize also degrades the accuracy of the (implicit) fourth order Gauss method, even though the Gauss methods can be shown to be unconditionally stable for variable step size; and, hence, linearized stability theory does not account for the poor performance of variable step size.

The second order Störmer method is usually written as

$$h^{-2}(y_{n+1} - 2y_n + y_{n-1}) = f(t_n, y_n).$$

This was proposed as an integrator for molecular dynamics by Verlet [8] together with the equation

$$\dot{y}_n = (y_{n+1} - y_{n-1})/2h$$

for purposes of "output." It can be shown [1] that this is equivalent to

(2)
$$\dot{y}_{n+\frac{1}{2}} = \dot{y}_n + \frac{h}{2} f(t_n, y_n),$$
$$y_{n+1} = y_n + h\dot{y}_{n+\frac{1}{2}},$$
$$\dot{y}_{n+1} = \dot{y}_{n+\frac{1}{2}} + \frac{h}{2} f(t_{n+1}, y_{n+1}).$$

The leapfrog method is obtained by omitting computations of $\dot{y}_n$ for integer values of $n$:

$$\dot{y}_{n+\frac{1}{2}} = \dot{y}_{n-\frac{1}{2}} + hf(t_n, y_n).$$

One step of the Störmer method (2) applied to the test equation (1) can be written

$$\begin{bmatrix} y_{n+1} \\ \omega^{-1}\dot{y}_{n+1} \end{bmatrix} = S \begin{bmatrix} y_n \\ \omega^{-1}\dot{y}_n \end{bmatrix} \quad \text{where } S = \begin{bmatrix} 1 - \frac{1}{2}(h\omega)^2 & h\omega \\ -h\omega + \frac{1}{4}(h\omega)^3 & 1 - \frac{1}{2}(h\omega)^2 \end{bmatrix}.$$

The product of the two eigenvalues of the matrix above, given by its determinant, is always one. It can be shown that the moduli of the two eigenvalues are both equal to 1 if and only if their sum, given by the trace of the matrix, is in the range $-2$ to 2, whence the necessity of the condition $h\omega < 2$ for stability. This is sufficient because it implies that the sum of the eigenvalues is strictly between $-2$ and 2, which means they must be imaginary and distinct. For different step sizes $h_1$ and $h_2$ the product of two such matrices will still have a determinant of 1 but a trace that could dip below $-2$ unless a condition more stringent than $h_n\omega < 2$ is imposed. For example with $h_1\omega = \frac{2}{3}$ and $h_2\omega = 2$ we get a trace of $-\frac{74}{27}$ for the matrix product. Attempts to imagine how this generalizes to more than two steps led eventually to the analysis in the paragraphs that follow.

The matrix $S$ has eigenvalues $e^{\pm i\theta}$ where $\theta = 2 \arcsin (h\omega/2)$ if we assume that $-2 < h\omega < 2$.

It is natural to regard the matrix $S$ as representing a rotation in phase space of $-\theta$ radians. With this in mind we obtain

$$S = DQD^{-1}$$

where

$$Q = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

and

$$D = \operatorname{diag}(1, \cos(\theta/2)).$$

Note that $\cos(\theta/2) > 0$. Also note that

$$S^n = DQ^nD^{-1} \tag{3}$$

where

$$Q^n = \begin{bmatrix} \cos n\theta & \sin n\theta \\ -\sin n\theta & \cos n\theta \end{bmatrix}.$$

To show the possibility of instability, we consider a sequence of $n_1$ steps of size $h_1$ followed by $n_2$ steps of size $h_2$. The purpose of $n_1$ and $n_2$ is to overcome any limit that we might care to impose on the step sizes. To show instability is equivalent to showing that the matrix

$$S_2^{n_2} \ S_1^{n_1}$$

has eigenvalues of moduli greater than 1, where $S_1$ and $S_2$ have the obvious meaning. The determinant of this matrix is just the product of the determinants of its factors, which is 1. Thus we must show that the trace can become less than $-2$ or greater than 2. Several lines of elementary manipulations beginning with (3) yield

$$\operatorname{trace}(S_2^{n_2} \ S_1^{n_1}) = 2\cos(n_1\theta_1 + n_2\theta_2) - \frac{(\cos\frac{1}{2}\theta_2 - \cos\frac{1}{2}\theta_1)^2}{\cos\frac{1}{2}\theta_2 \cos\frac{1}{2}\theta_1} \sin n_2\theta_2 \sin n_1\theta_1 \tag{4}$$

where $\theta_1$ and $\theta_2$ have the obvious meaning. Now choose $h_1$, $h_2$, $n_1$, and $n_2$ so that

$$n_1\theta_1 + n_2\theta_2 = \pi \quad \text{and} \quad \theta_1 \neq \theta_2.$$

Then the first term of (4) is $-2$ and the second term is negative. The above choice is possible regardless of any (nonpathological) restriction placed on step sizes or step size ratios.

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