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LETTER TO THE EDITOR

Comments on "Numerical Instability due to Varying Time Steps in Explicit Wave Propagation and Mechanics Calculations" by Joseph P. Wright[1]

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I am writing to point out additional relevant results on this topic.

The loss of stability for the leapfrog method (explicit central difference time integration) when the time step is varied is discussed in [3]. It is shown there for the test equation $\ddot{u} = -\omega^2 u$ that there does not exist a positive value $p_{\max}$ such that restricting the time step Δt_n by $\omega \Delta t_n < p_{\max}$ ensures stability. Nor can stability be guaranteed if we also impose a restriction on the time step ratios of the form $a < \Delta t_{n+1}/\Delta t_n < b$, where $a < 1 < b$. To demonstrate instability, it is enough to consider n_1 steps of length Δt_1, followed by n_2 steps of length Δt_2, for which one can obtain an explicit expression for the trace of the amplification matrix. It can be shown that this trace will be less than -2 if we choose

$$2n_1 \arccos \frac{\omega \Delta t_1}{2} + 2n_2 \arccos \frac{\omega \Delta t_2}{2} = \pi, \quad \Delta t_1 \neq \Delta t_2.$$

Method (A.1) explored in the Appendix of the Wright article occurs in the literature [6] under the name LIM2. As the author observes, it does not satisfactorily deal with variable stepsize. A method that does is the implicit midpoint method, for which the amplification matrix is an orthogonal matrix. Of course, it has the same practical drawback of implicitness as does LIM2. (Also, the implicit midpoint has two times the error of leapfrog and LIM2 has five times the error [5].)

Practical solutions to the problem of variable stepsize have been proposed in literature on reversible and symplectic integration, e.g., [2, 1, 4].

[1] J. P. Wright, *J. Comput. Phys.* **140**, 421 (1998).

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REFERENCES

1. E. Hairer, Variable time step integration with symplectic methods, *Appl. Numer. Math.* **25**(2–3), 219 (1997).
2. W. Huang and B. Leimkuhler, The adaptive Verlet method, *SIAM J. Sci. Comput.* **18**, 239 (1997).
3. R. D. Skeel, Variable step size destabilizes the Störmer/leapfrog/Verlet method, *BIT* **33**, 172 (1993).
4. R. D. Skeel and J. J. Biesiadecki, Symplectic integration with variable stepsize, *Ann. Numer. Math.* **1**, 191 (1994).
5. R. D. Skeel, G. Zhang, and T. Schlick, A family of symplectic integrators: Stability, accuracy, and molecular dynamics applications, *SIAM J. Sci. Comput.* **18**(1), 203 (1997).
6. G. Zhang and T. Schlick, Implicit discretization schemes for Langevin dynamics, *Mol. Phys.* **84**, 1077 (1995).