

We next combine (3.75a) and (3.75c) for the momentum coordinate and (3.75b) and (3.75d) for the position and obtain

$$p_i^{(2)} = p_i^{(0)} + (F_i^{(0)} + F_i^{(1)})\delta t \quad (3.76a)$$

$$q_i^{(2)} = q_i^{(0)} + 2p_i^{(1)}\delta t. \quad (3.76b)$$

We take $\delta t = \Delta t/2$ and combine (3.76b) with (3.75a) and find

$$p_i^{(2)} = p_i^{(0)} + \frac{1}{2}(F_i^{(0)} + F_i^{(1)})\Delta t \quad (3.77a)$$

$$q_i^{(2)} = q_i^{(0)} + p_i^{(0)}\Delta t + \frac{1}{2}F_i^{(0)}(\Delta t)^2, \quad (3.77b)$$

which is identical to the Verlet algorithm (3.48), because for unit mass the force and acceleration are equal.

Reversing the order of the updates for the coordinates and the momenta also leads to symplectic algorithms:

$$q_i^{(k+1)} = q_i^{(k)} + b_k \delta t p_i^{(k)} \quad (3.78a)$$

$$p_i^{(k+1)} = p_i^{(k)} + a_k \delta t F_i^{(k+1)}. \quad (3.78b)$$

A third variation uses (3.74) and (3.78) for different values of k in one algorithm. Thus, if $M = 2$, which corresponds to two intermediate calculations per time step, we could use (3.74) for the first intermediate calculation and (3.78) for the second.

Why are these algorithms important? Because of the symplectic property, these algorithms will simulate an exact Hamiltonian, although not the one we started with in general (see Problem 3.1c, for example). However, this Hamiltonian will be close to the one we wish to simulate if the a_k and b_k are properly chosen. Second, these algorithms are frequently more accurate and stable than nonsymplectic algorithms. Finally, for even values of M , the algorithms are time-reversible invariant, which is a property of the actual systems we are trying to simulate. Examples and comparisons for various algorithms are given in the paper by Gray et al.

REFERENCES AND SUGGESTIONS FOR FURTHER READING

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