Numerical Analysis in Molecular Dynamics

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1 What's the best time step in MD?

Last quarter, we finished the assignment of molecular dynamics and got a general understanding of how it works by making comments and deriving formulas for the code, but there are some concerns about the default parameters especially the time step Δt, which has a important impact in the simulation.

Considering the Taylor series in the derivation of $x(t)$ and $v(t)$. Here, we only use the first three terms and ignore the rest remaining terms. Although, the Δt is so tiny that we can omit these terms with high power, and the truncation error is acceptable. But how can we know the truncation error won't be accumulated step by step, because there are millions of particles with millions steps. Theoretically, I am afraid that the initial tiny error will result in dramatic error like butterfly effect. u_0 For the Verlet integrator, we have

$$x(t+\Delta t) = x(t) + \frac{dx(t)}{dt}\Delta t + \frac{1}{2}\frac{d^2x(t)}{dt^2}(\Delta t)^2 + \frac{1}{6}\frac{d^3x(t)}{dt^3}(\Delta t)^3 + ... \tag{1}$$

$$x(t-\Delta t) = x(t) - \frac{dx(t)}{dt}\Delta t + \frac{1}{2}\frac{d^2x(t)}{dt^2}(\Delta t)^2 - \frac{1}{6}\frac{d^3x(t)}{dt^3}(\Delta t)^3 + ... \tag{2}$$

then, equation (11) - (12) yields

$$v(t) = \frac{x(t+\Delta t) - x(t-\Delta t)}{2\Delta t} - \frac{x^{(3)}(\xi)}{6}(\Delta t)^3 \tag{3}$$

Where $v(t) = \frac{dx}{dt}$, and $\xi \in (t-\Delta t, t+\Delta t)$.

However, beyond the truncation error, it is also necessary to attach more importance to round-off error when approximating derivatives with numerical method in computer. Suppose that in evaluating $x(t+\Delta t)$ and $x(t-\Delta t)$, we are encountering round-off errors

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$e(t+\Delta t)$ and $e(t-\Delta t)$. Then the computer actually uses the values $\tilde{x}(t+\Delta t)$ and $\tilde{x}(t-\Delta t)$, which are related to the true values $x(t+\Delta t)$ and $x(t-\Delta t)$ by

$$x(t+\Delta t) = \tilde{x}(t+\Delta t) + e(t+\Delta t) \tag{4}$$

$$x(t-\Delta t) = \tilde{x}(t-\Delta t) + e(t-\Delta t) \tag{5}$$

As a result, the total error in the approximation

$$x^{'}(t) - \frac{x(t+\Delta t) - x(t-\Delta t)}{2\Delta t} = \frac{e(t+\Delta t) - e(t-\Delta t)}{2\Delta t} - \frac{x^{(3)}(\xi)}{6}(\Delta t)^3 \tag{6}$$

If we assume that the round-off errors $e(t \pm \Delta t)$ are bounded by some number $\varepsilon > 0$, and the third derivative of $x(t)$ is bounded by a number $M > 0$, then we may have this ineuqality

$$\left| x^{'}(t) - \frac{x(t+\Delta t) - x(t-\Delta t)}{2\Delta t} \right| \leq \frac{\varepsilon}{\Delta t} + \frac{(\Delta t)^2}{6} M \tag{7}$$

The total error is both related to round-off error, the first term, and truncation error, the second term. To reduce the truncation error $\frac{(\Delta t)^2}{6}M$, we need to reduce the timestep Δt. However, as Δt is reduced, the first term $\frac{\varepsilon}{\Delta t}$ will grow, in that case the round-off error will dominate the calculations.

In summary, it seems not always correct to make the calculation increasingly accurate by making the timestep very small.