Langevin dynamics modified Velocity Verlet algorithm

Martin Kröger[1]

[1] *Department of Materials, Polymer Physics, ETH Zurich, CH–8093 Zurich, Switzerland*
http://www.complexfluids.ethz.ch

Notation: Time step Δ, position r, velocity v, force $f = f(r)$, half time step $\Delta' = \Delta/2$ and mass is set to unity. The equations hold for any dimension separately. Create an initial r, initial v, and calculate $f = f(r)$. Each subsequent time step does the following.

Classical Velocity Verlet algorithm

$$\begin{aligned} v &= v + \Delta' f, \\ r &= r + \Delta v, \\ &\text{calculate } f = f(r) \\ v &= v + \Delta' f \end{aligned} \tag{1}$$

typically supplemented by a temperature T control ensuring $\langle v^2 \rangle = k_\mathrm{B} T$.

Langevin Modified Velocity Verlet algorithm

with particle friction coefficient ζ and at temperature T.

$$\begin{aligned} &\text{choose } \eta \text{ from } \langle \eta \rangle = 0,\ \langle \eta^2 \rangle = 1 \\ v &= v + \Delta' f + b\eta, \\ r &= r + cv, \\ &\text{calculate } f = f(r) \\ v &= av + b\eta + \Delta' f, \end{aligned} \tag{2}$$

where we abbreviated the constants

$$a = (2 - \zeta\Delta)/(2 + \zeta\Delta), \tag{3}$$

$$b = \sqrt{k_\mathrm{B} T \zeta \Delta'}, \tag{4}$$

$$c = 2\Delta/(2 + \zeta\Delta) \tag{5}$$

Comments

The modified algorithm 2 does not require a temperature control and reduces to the classical algorithm 1 for the frictionless case of $\zeta = 0$ implying $a = 1$, $b = 0$, $c = \Delta$. The modified algorithm requires a single independent normal distributed random number η for each coordinate and each time step. In the absence of forces, $f = 0$, the modified algorithm simplifies to $r = r + c(v + b\eta)$ and

$$v = av + \frac{bc}{\Delta'}\eta \tag{6}$$

If we begin with $v_0 = 0$, and then repeat calculating new velocities $v_{1,2,..,M}$ using eq 6 iteratively, we ultimately generate a Gaussian distributed set of v values with the feature

$$\langle v \rangle = 0, \qquad \langle v^2 \rangle = k_\mathrm{B} T \tag{7}$$

irrespective the precise value for ζ as long as $\zeta > 0$ and thus $a < 1$. Proof:

$$\begin{aligned} \langle v^2 \rangle &= \frac{1}{M} \sum_{j=0}^{M-1} v_j^2 \\ &= \frac{4b^2c^2}{M\Delta^2} \sum_{j=0}^{M-1} a^{2j}(M - 1 - j) \\ &= \frac{4b^2c^2}{M\Delta^2} \frac{a^{2M} + M(1 - a^2) - 1}{(1 - a^2)^2} \end{aligned} \tag{8}$$

and thus

$$\lim_{M\to\infty} \langle v^2 \rangle = \frac{4b^2c^2}{(1 - a^2)\Delta^2} = k_\mathrm{B} T \tag{9}$$

For larger ζ, the more quickly is the Gaussian approached. For this calculation we assumed $v_0 = 0$. In any case the initial value v_0 becomes irrelevant in the limit $M \to \infty$.

[1] M. Kröger, Models for polymeric and anisotropic liquids (Springer, Berlin, 2005)