1 Langevin Equation

We wish to devise an algorithm for the Langevin equation

$$m\frac{dv}{dt} = F(r(t)) - \gamma v(t) + \alpha\eta(t)$$

We consider a discrete-time dynamics with time step Δt.
We first consider a time s with $t < s < t + \Delta t$, and integrate the Langevin equation obtaining

$$m\int_t^s dp\, \dot{v}(p) = \int_t^s dp\, [F(r(p)) - \gamma v(p) + \alpha\eta(p)]$$

so that

$$v(s) = v(t) + \frac{1}{m}\int_t^s dp\, F(r(p)) - \frac{\gamma}{m}\int_t^s dp\, v(p) + \frac{\alpha}{m}W(s-t). \tag{1}$$

Now, we integrate in s from t up to $t + \Delta t$:

$$\int_t^{t+\Delta t} ds v(s) = v(t)\Delta t + \int_t^{t+\Delta t} ds \left[\frac{1}{m}\int_t^s dp\, F(r(p)) - \frac{\gamma}{m}\int_t^s dp\, v(p) + \frac{\alpha}{m}W(s-t)\right].$$

which gives ($F(p) = F(r(p))$ as usual)

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \int_t^{t+\Delta t} ds \left[\frac{1}{m}\int_t^s dp\, F(p) - \frac{\gamma}{m}\int_t^s dp\, v(p)\right] + \frac{\alpha}{m}u(\Delta t).$$

Up to now, everything is exact. We wish now to perform an approximation with an error of order Δt^3. We use the simplest approximation for the two integrals:

$$\int_t^{t+\Delta t} ds \int_t^s dp\, F(p) = \int_t^{t+\Delta t} ds \int_t^s dp[F(t) + O(\Delta t)] = \frac{1}{2}\Delta t^2 F(t) + O(\Delta t^3).$$

and

$$\int_t^{t+\Delta t} ds \int_t^s dp\, v(p) = \int_t^{t+\Delta t} ds \int_t^s dp[v(t) + O(\Delta t)] = \frac{1}{2}\Delta t^2 v(t) + O(\Delta t^3).$$

We thus obtain the recursion

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{1}{2m}F(t)\Delta t^2 - \frac{\gamma}{2m}v(t)\Delta t^2 + \frac{\alpha}{m}u(\Delta t)$$

which generalizes the usual Verlet formula. No approximation has been made on the noise term.
We also need a recursion relation for the velocity. We go back to the exact expression (1) and set $s = t + \Delta t$.

$$v(t+\Delta t) = v(t) + \frac{1}{m}\int_t^{t+\Delta t} dp\, F(r(p)) - \frac{\gamma}{m}\int_t^{t+\Delta t} dp\, v(p) + \frac{\alpha}{m}W(\Delta t).$$

The velocity integral can be don exactly:

$$\int_t^{t+\Delta t} dp\, v(p) = r(t+\Delta t) - r(t).$$

The integral over the force is treated as in the standard Verlet case, so that the neglected terms are of order Δt^3:

$$\int_t^{t+\Delta t} dp\, F(r(p)) = \frac{\Delta t}{2}[F(t+\Delta t) + F(t)].$$

Therefore, we obtain the recursion

$$v(t+\Delta t) = v(t) + \frac{\Delta t}{2m}[F(t+\Delta t) + F(t)] - \frac{\gamma}{m}[r(t+\Delta t) - r(t)] + \frac{\alpha}{m} W(\Delta t).$$

We now discuss the practical implementation. Suppose we have computed $r(t)$, $v(t)$ and $F(t) = F(r(t))$. We wish to compute the same quantities at time $t + \Delta t$. We proceed as follows:

- 1) we compute the independent Gaussian random number with zero mean and unit variance ξ and θ and set

$$W(\Delta t) = \sqrt{\Delta t}\xi \qquad u(\Delta t) = \frac{1}{2}(\Delta t)^{3/2}\left(\xi + \frac{1}{\sqrt{3}}\theta\right);$$

- 2) we compute the new position using

$$r(t+\Delta t) = r(t) + v(t)\Delta t + \frac{1}{2m}F(t)\Delta t^2 - \frac{\gamma}{2m}v(t)\Delta t^2 + \frac{\alpha}{m}u(\Delta t);$$

- 3) we compute the force $F(t+\Delta t)$;
- 4) we compute the new velocity:

$$v(t+\Delta t) = v(t) + \frac{\Delta t}{2m}[F(t+\Delta t) + F(t)] - \frac{\gamma}{m}[r(t+\Delta t) - r(t)] + \frac{\alpha}{m} W(\Delta t).$$