— HOMEWORK 4 —
— LANGEVIN DYNAMICS —

Given equations:

$$ma(t) = F(r,t) - \gamma m v(t) + R(t) \quad \text{---} \quad (1)$$

$$R(t) = Z(t) . \sqrt{2 k_B T . \gamma m / \Delta t} \quad \text{---} \quad (2)$$

$$v(t+\frac{1}{2}\Delta t) = v(t) + \left[\frac{1}{m}\left[F(r(t),t) + R(t)\right] - \gamma v(t)\right]\frac{\Delta t}{2} \quad \text{--} \quad (3)$$

$$r(t+\Delta t) = r(t) + v\left(t+\frac{1}{2}\Delta t\right)\Delta t \quad \text{---} \quad (4)$$

$$v(t+\Delta t) = \left[v(t+\frac{1}{2}\Delta t) + \frac{F(r(t+\Delta t), t+\Delta t) + R(t+\Delta t)}{m}\frac{\Delta t}{2}\right]\frac{1}{1+\gamma\frac{\Delta t}{2}} \quad (5)$$

$$a(t) = \frac{F(r,t) + R(t)}{m} - \gamma v(t) \quad \text{---} \quad (6)$$

$$\bar{a}(t+\Delta t) = \frac{F(r(t+\Delta t), t+\Delta t) + R(t+\Delta t)}{m} \quad \text{---} \quad (7)$$

Exercise 1:

a) $$v(t+\frac{1}{2}\Delta t) = v(t) + \underbrace{\left[\frac{1}{m}\left[F(r(t),t) + R(t)\right] - \gamma v(t)\right]}_{a(t)}\frac{\Delta t}{2}$$

$$v(t+\frac{1}{2}\Delta t) = v(t) + a(t) . \frac{\Delta t}{2} \quad \rightarrow \text{Modified Equation 3!}$$
(v- halftime)

$$r(t+\Delta t) = r(t) + v(t+\frac{1}{2}\Delta t)$$
(r- fut)
$$= r(t) + v(t) + a(t) . \frac{\Delta t}{2} \quad \rightarrow \text{Modified Equation 4!}$$

Equations

$$v(t+\Delta t) = \left[v\left(t+\frac{1}{2}\Delta t\right) + \underbrace{\frac{F(r(t+\Delta t), t+\Delta t) + R(t+\Delta t)}{m}}_{\tilde{a}(t+\Delta t)} \frac{\Delta t}{2} \right] \frac{1}{1+\gamma \frac{\Delta t}{2}}$$

$$v(t+\Delta t) = \left[\underbrace{v\left(t+\frac{1}{2}\Delta t\right)}_{\text{v-halftime}} + \tilde{a}(t+\Delta t) \cdot \frac{\Delta t}{2} \right] \cdot \frac{1}{1+\gamma \frac{\Delta t}{2}}$$

$$\underbrace{v(t+\Delta t)}_{\text{v-fut.}} = \left[V(t) + a(t) \cdot \frac{\Delta t}{2} + \tilde{a}(t+\Delta t) \cdot \frac{\Delta t}{2} \right] \cdot \frac{1}{1+\gamma \frac{\Delta t}{2}}$$

→ modified Equation S.

- The difference about these equations than the equations we used in our implementation of the velocity verlet algorithm is that we have new terms in the equations (drag and random perturbations)

When we used velocity Verlet algorithm to numerically solve classical equations of motion for bond vibration for an isolated CO molecule, we assume that there is no exchange of matter or energy between the single CO molecule system and its surroundings. In this exercise, we modify velocity Verlet code to implement the BBK algorithm. Actually, we use our code to simulate the bond vibration of CO molecule experiencing drag and random perturbations. (Newton's second law for accelaration to include drag as well as random perturbations to the force)

$$ma(t) = F(r,t) \underbrace{- \gamma m v(t)}_{\text{"drag" or "friction"}} + \underbrace{R(t)}_{\text{Random perturbation}}$$

$\hookrightarrow = Z(t) \cdot \sqrt{2 k_B T \gamma M / \Delta t}$

- Verlet velocity:

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{1}{2}\left(\vec{a}(t) + \vec{a}(t+\Delta t)\right).\Delta t$$

$$\boxed{\text{v\_fut} = \text{v\_curr} + 0.5 * \text{a\_curr} * dt + 0.5 * \text{a\_fut} * dt} \quad \text{Equation } (1)$$

- BBK algorithm:

$$v(t+\Delta t) = \left[\underbrace{v\left(t+\frac{1}{2}\Delta t\right)}_{v(t)+a(t).\Delta t/2} + \underbrace{\frac{F(r(t+\Delta t), t+\Delta t) + \overset{0}{\cancel{R(t+\Delta t)}}}{m}}_{a(t+\Delta t)} . \frac{\Delta t}{2}\right] . \frac{1}{1+\underbrace{\gamma}_{\gamma=0}\frac{\Delta t}{2}}$$

$$v(t+\Delta t) = \left[v(t) + a(t).\frac{\Delta t}{2} + a(t+\Delta t).\frac{\Delta t}{2}\right] . \frac{1}{1+0}$$

$$v(t+\Delta t) = v(t) + a(t).\frac{\Delta t}{2} + a(t+\Delta t).\frac{\Delta t}{2}$$

$$\boxed{\text{v\_fut} = \text{v\_curr} + 0.5 * \text{a\_curr} * dt + 0.5 * \text{a\_fut} * dt} \quad \text{Equation } (2)$$

When $\gamma = 0$ and $R(t) = 0$ → BBK algorithm

$$\Big\downarrow \text{reduce/equations}$$

Velocity Verlet algorithm

Equation 1 = Equation 2