Equation 3

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

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

$$v\left(t+\tfrac{1}{2}\Delta t\right) = v(t) + a(t)\frac{\Delta t}{2} \quad \text{...New equation 3}$$

Equation 4

$$r(t+\Delta t) = r(t) + v\left(t+\tfrac{1}{2}\Delta t\right)\Delta t$$

$$r(t+\Delta t) = r(t) + v(t) + a(t)\frac{1}{2}\Delta t \quad \text{... New equation 4}$$

Equation 5

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

$$v(t+\Delta t) = \left[v(t) + a(t)\cdot\frac{\Delta t}{2} + a(t+\Delta t)\frac{\Delta t}{2}\right]\cdot\frac{1}{1+\gamma\frac{\Delta t}{2}} \quad \text{...New equation 5}$$

The difference in these equations is that they contain "new terms" (drag and random perturbations).

When $\gamma = 0$ and $R(t) = 0$

$$\text{BBK}: \quad v(t+\Delta t) = v(t) + a(t)\frac{\Delta t}{2} + \frac{F(r(t+\Delta t),t+\Delta t) + \overbrace{R(t+\Delta t}^{0}}{m}\frac{\Delta t}{2}\cdot\frac{1}{1+\gamma\frac{\Delta t}{2}}$$

$$v(t+\Delta t) = v(t) + a(t)\frac{\Delta t}{2} + a(t+\Delta t)\frac{\Delta t}{2}\cdot\frac{1}{1+0}$$

$$v\_fut = v\_curr + 0.5 * a\_curr * dt + 0.5 * a\_fut * dt$$

verlet velocity:

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

$$v\_fut = v\_curr + 0.5 * a\_curr * dt + 0.5 * a\_fut * dt$$

Using BBK DOES reduce equations implementing the velocity verlet algorithm

when $r=0$ and $R(t)=0$.

Exercise 2:

DONE, in Github as "BBK"

Exercise 3:

The bond length vs time trajectory changed. The energies seem to converge at the same temperature used in simulations.

Exercise 4:

If you decrease the gamma, all trajectories change significantly. Lower gamma gave a lower mean temp. for last 1000 time steps but increased for the next 1000 time steps.