

# REPORT

## ASSIGNMENT 3, BD SIMULATION

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#### Problem statement

In this assignment we were required to plot the dimensionless distance between the 2 beads of the dumbbell model of the polymer as a function of dimensionless time and also the rms value of the separation.

#### Solution

The code in the last assignment was for one isolated particle dispersed in a medium. In this assignment we modelled an isolated polymer chain as a dumbbell with 2 beads by slightly modifying the previous code by including the force due to the spring. Now three forces act on each bead.

#### Dynamics of a single polymer chain

Drag force on each bead  $\vec{F}_{drag,i} = -\zeta \vec{u}_i = -\zeta \frac{d\vec{r}_i}{dt}$

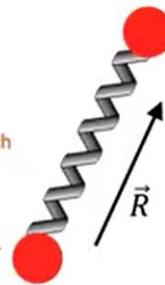
Brownian force on each bead  $\vec{F}_{B,i} = \sqrt{\frac{6k_B T \zeta}{\Delta t}} \vec{n}_i$

$\vec{n}_i = \begin{bmatrix} n_{x,i} \\ n_{y,i} \\ n_{z,i} \end{bmatrix}$ ; Each component is a random number between -1 and 1

Spring force  $\vec{F}_{sp,1} = \frac{k_B T (3 - \hat{r}^2)}{v b_K^2 (1 - \hat{r}^2)} \vec{R}$

$\vec{F}_{sp,2} = -\frac{k_B T (3 - \hat{r}^2)}{v b_K^2 (1 - \hat{r}^2)} \vec{R}$        $\vec{R} = \vec{r}_2 - \vec{r}_1$        $\hat{r} = \frac{|\vec{R}|}{v b_K}$

$v$ : number of Kuhn lengths mimicked by one spring  
 $b_K$ : Kuhn length of the polymer chain



#### Equation of Motion ( $i = 1, 2$ )

$0 = \vec{F}_{B,i} + \vec{F}_{drag,i} + \vec{F}_{sp,i}$        $\zeta \frac{d\vec{r}_i}{dt} = \sqrt{\frac{6k_B T \zeta}{\Delta t}} \vec{n}_i + \vec{F}_{sp,i}$



We solve the dimensionless equation of motions, using similar approach as done in previous 2 assignments.

### Solving equations of motion of beads

**Equation of Motion**

$$\zeta \frac{d\vec{r}_i}{dt} = \sqrt{\frac{6k_B T \zeta}{\Delta t}} \vec{n}_i + \vec{F}_{sp,i}$$

Use non-dimensional version:

$$\frac{d\vec{r}_1^*}{dt^*} = \sqrt{\frac{6}{\Delta t^*}} \vec{n}_1 + \frac{3 - \hat{r}^2}{v(1 - \hat{r}^2)} \vec{R}^*$$

$$\frac{d\vec{r}_2^*}{dt^*} = \sqrt{\frac{6}{\Delta t^*}} \vec{n}_2 - \frac{3 - \hat{r}^2}{v(1 - \hat{r}^2)} \vec{R}^*$$

Select a length scale equal to Kuhn step:  $b_K$

$$r^* = \frac{r}{b_K}$$

A relevant time scale:  $\frac{\zeta b_K^2}{k_B T}$

$$t^* = \frac{t}{\frac{\zeta b_K^2}{k_B T}} = t \frac{k_B T}{\zeta b_K^2}$$

Force scale  $\frac{k_B T}{b_K}$

$$F^* = \frac{F}{k_B T / b_K} = \frac{F b_K}{k_B T}$$

## CODE OUTPUT

RMS VALUE IS :  
21.1698

## Plot

