

Brownian Dynamics Simulation Package

AJS-wlcsim

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2/3/15

Abstract

This Brownian dynamics simulation package is a basic beaded-chain polymer simulation to model a discrete wormlike chain polymer (stretchable). The elastic energy includes a stretching and bending energy. There is an option to enforce a fixed chain length through a Lagrange constraint.

Polymer model

The total energy of the polymer is given by

$$E_{tot} = E_{stretch} + E_{bend} \quad (1)$$

The stretching energy $E_{stretch}$ is given by

$$E_{stretch} = \frac{A}{2} \sum_{n=1}^{N-1} (b_n - l_0)^2 \quad (2)$$

where A is the stretching modulus, $b_n = |\vec{r}_{n+1} - \vec{r}_n|$, and l_0 is the equilibrium length between beads. The bending energy E_{bend} is given by

$$E_{bend} = \frac{B}{2} \sum_{n=1}^{N-2} (\vec{u}_{n+1} - \vec{u}_n)^2 = B \sum_{n=1}^{N-2} (1 - \vec{u}_{n+1} \cdot \vec{u}_n) \quad (3)$$

where B is the bending modulus, and $\vec{u}_n = (\vec{r}_{n+1} - \vec{r}_n)/b_n$ is the unit tangent vector.

Input file

The following input file can be copied directly from the latex source file.

```
! -----  
!  
!Input file for polymer simulation package  
  
!-Record 1  
!  
!  KAP                      Compression modulus  
500.  
  
!-Record 2  
!  
!  EPS                      Bending modulus  
21.2  
  
!-Record 3  
!  
!  L0                      Equilibrium segment length  
1.  
  
!-Record 4  
!  
!  XI                      Drag coefficient  
1.  
  
!-Record 5  
!  
!  N                      Number of beads
```

50

!-Record 6

! TF Total simulation time

1.

!-Record 7

! INDMAX Total number of save points

100

!-Record 8

! DT Timestep for integration

0.0002

!-Record 9

! FRMFILE Load in the initial conf?

0

!-Record 10

! BROWN Include Brownian forces?

1

!-Record 11

! CON Include length constraint?

1

! -----