Brownian Dynamics Simulation Package

AJS-wlcsim

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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

$$E_{tot} = E_{stretch} + E_{bend} \tag{1}$$

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

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

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

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

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 inital conf?
 0

!-Record 10
!  BROWN           Include Brownian forces?
 1

!-Record 11
!  CON             Include length constraint?
 1

! ------------------------------------------------
```