Main codes: active\_polymer\_adsorption.f

Langevin dynamics simulation of end-grafted active polymer chain. It was written in Fortran 90. Detailed simulation methods can be found in the following cites:

(1) M. B. Luo and Y. F. Shen, Langevin dynamics simulations for the critical adsorption of end-grafted active polymers, Soft Matter, 2024, 20, 5113–5121.

(2) Y. F. Shen and M. B. Luo, Knotting and adsorption of end-grafted active polymers, Soft Matter, submitted.

Usage：

Windows: active\_polymer\_adsorption.exe

Linux: ./active\_polymer\_adsorption.X

Format of input file “parameters\_input.txt”

'n65k0f2Dr3s3' output file names

0 'x.cfg' if the first number is 1, then read in initial conformation

200 Number of samples

60.0d0 60.0d0 40.0d0 system size x y z

1 65 number of polymer chain and length (the first bead is active bead)

1.0d0 bead size

30.0d0 FENE strength

1.5d0 1.2d0 maximum FENE bond for passive part and the first bond connected the active bead

0.0d0 0.0d0 Bending strength and equilibrium bond angle

1.0d0 1.12d0 WCA potential

2.0d0 Active force Fa

3.0d0 1.0d0 Diffusion coefficients D\_r and D\_t

0.1d0 Rotational inertia J

1.0d0 temperature of solvent

0.005d0 timestep for Langevin dynamics

2000 20000 500 500 Equilibrium time, Statistical time, Time for recording conformation, Time for output conformation

3 suface type

2.5d0 rcut for polymer-surface

1 36 Number of polymer-surface interaction Eps (starting No and ending No)

0.05 0.1 0.15 0.2 0.3 0.4 0.5 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95 1.0 1.05 1.1 1.15 1.2 1.25 1.3 1.35 1.4 1.45 1.5 1.6 1.7 1.8 1.9 2.0 2.2 2.4 2.6 2.8 3.0 Interaction strength for simulation

Every energy has its own conformation file with suffix 00xx

Output:

1. Data file:

Format:

“Eps” “mean-square end-to-end distance R^2” “surface normal component of mean-square end-to-end distance R^2\_z” “mean-square radius of gyration R\_G^2” “surface normal component of mean-square radius of gyration R\_G^2\_z” “mean height of mass center of polymer chain z\_c” “mean bond length” “two-dimensional shape parameter A\_2D” “mean number of adsorbed monomer M” “mean square M” “mean interaction energy between polymer and surface E” “mean square E”

1. Conformation file:

Record coordinates of the whole polymer chain

Format:

[serial](https://cn.bing.com/dict/search?q=serial&FORM=BDVSP6&cc=cn) [number](https://cn.bing.com/dict/search?q=number&FORM=BDVSP6&cc=cn) polymer ID monomer ID x y z monomer species