

# Assembly documentation

Francisco Javier Vázquez Tavares

## Contents

1	Description of the simulation . . . . .	1
1.1	Potentials . . . . .	1
1.2	LAMMPS implementation . . . . .	2
	References	3

## 1 Description of the simulation

The simulation methodology is based on (1) and (2), with the objective of create a polymer structure of a hydro-gel and characterize its rheological properties. This methodology creates a hydro-gel structure by creating a interaction between two types of patchy particles. One type of patchy particle represent a Crosslinker and is define with 5 particles, one at the center and the rest are placed in the vertices of a tetrahedron that circumscribes the center particle. The other type of patchy particle represent a Monomer and is define with 3 particles, on at the center and the rest are placed at the poles of the center particle with an 180 degrees between them. Prior to describe with detail the methodology, it is important mention that to from now on I will refer to the center particle of the Crosslinker patchy particle as “CL” and the particles around CL as “PA”. Naturally, the center particle of the Monomer patchy particle as “MO” and the particles around MO as “PB”.

The proposed methodology to create hydro-gels considers that the geometry of the position of the PA and PB are the same in all the patchy particles and does not change during the simulation. Also, takes into account the following interactions:  $CL \longleftrightarrow MO$ ,  $PA \longleftrightarrow PB$ ,  $PB \longleftrightarrow PB$ . The  $CL \longleftrightarrow MO$  interaction is repulsive, and the  $PA \longleftrightarrow PB$ ,  $PB \longleftrightarrow PB$  interactions are attractive. However, the main difference between the articles cited and the simulations implemented is the absence of FENE bonds and Swelling potential.

### 1.1 Potentials

$$U_{WCA}(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] + \epsilon, \quad r \in [0, 2^{1/6}\sigma] \quad (1)$$

$$U_{\text{patchy}}(r_{\mu\nu}) = 2\epsilon_{\mu\nu} \left( \frac{\sigma_p^4}{2r_{\mu\nu}^4} - 1 \right) \exp \left[ \frac{\sigma_p}{(r_{\mu\nu} - r_c) + 2} \right], \quad r_{\mu\nu} \leq r_c \quad (2)$$

$$U_{\text{swap}}(r) = w \sum_{\lambda, \mu, \nu} \epsilon_{\mu\nu} U_3(r_{\lambda, \mu}) U_3(r_{\lambda, \nu}) \quad (3)$$

$$U_3 = -U_{\text{patchy}}(r)/\varepsilon_{\mu\nu} \quad (4)$$

## 1.2 LAMMPS implementation

# References

1. N. Gnan, L. Rovigatti, M. Bergman, E. Zaccarelli, *Macromolecules* **50**, 8777–8786, ISSN: 0024-9297, 1520-5835 (Nov. 2017).
2. V. Sorichetti *et al.*, *The Journal of Chemical Physics* **158**, 074905, ISSN: 0021-9606, 1089-7690 (Feb. 2023).