A new Approach to DPD Repulsion Parameter Estimation

Felix Bänsch [1,3], Mirco Daniel [1], Harald Lanig [2], Christoph Steinbeck [3], Achim Zielesny [1]

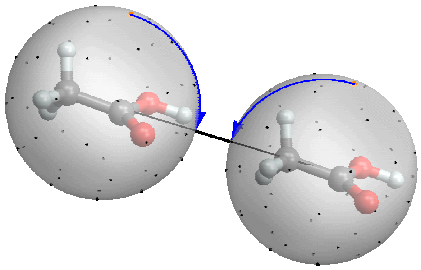
1 Institute for Bioinformatics and Cheminformatics, Westphalian University of Applied Sciences, Recklinghausen, Germany

2 Department of Chemistry and Pharmacy, Friedrich-Alexander University, Erlangen-Nürnberg, Germany

3 Institute for Inorganic and Analytical Chemistry, Friedrich-Schiller University, Jena, Germany

Dissipative Particle Dynamics (DPD) is a mesoscopic simulation technique for complex fluids and soft matter systems. Molecular Fragment DPD is a "bottom-up" variant with particles being defined as small "fragment molecules" with a molecular weight in the order of 100 Da. Larger molecules are then partitioned into adequate smaller "fragment molecule" particles that are bonded by harmonic springs to mimic covalent connectivities and spatial 3D conformations. The conservative interaction between two DPD particles i and j is characterized by an isotropic repulsion a_{ij} [1].

This project aims at a new force field based approach for consistent a_{ij} parameter estimation to obtain a "fragment molecule" particle set especially for biomolecular simulations that contain peptides and proteins.



The a_{ij} parameters are themselves determined by a coordination number Z_{ij}, i.e. the average number of particles i around a particle j, and the differential pair interaction energy ΔE_{ij} of the particle pair so that strategies for approximation of the latter two are under investigation.

Final goal is an open protocol for automated a_{ij} parameter estimation that utilizes the Wolfram Language of the Mathematica platform [2] as a math-enabled scripting engine where all force field related molecular mechanics and dynamics calculations are to be performed with the open TINKER package [3].

[1] R. D. Groot, P. B. Warren, J. Chem. Phys., 1997, 107, 4423
[2] Wolfram Mathematica: https://www.wolfram.com/mathematica/
[3] J. Rackers *et al.*, J. Chem. Theory Comput., 2018, 14, 5273