Department of Physics and Astronomy
Heidelberg University

Bachelor Thesis in Physics
submitted by

Gabriel Scherer

born in Mainz (Germany)

2003

About ...

This Bachelor Thesis has been carried out by Gabriel Scherer at the

Institute for theoretical Physics in Heidelberg
under the supervision of
Prof. Tristan Bereau

Contents

Abstract

1 Introduction

Coarse-grained (CG) molecular dynamic (MD) models are a very effective to simulate large molecular systems. Unlike all atom simulation which aim to simulate the trajectories of every atom, the idea is to substitute groups of atoms by a bead which is given properties that match the corresponding atoms.

Using this CG approach has the benefits of much lower computational costs which makes it viable to simulate large systems that would be unattainable for a all atoms simulation. The most popular method for CG molecular dynamics is the MARTINI model with the Lennard-Jones potential as the underlying force-field.

In this paper I will use the MARTINI method as a baseline for a system but then apply a different force-field **dissipative particle dynamics** (DPD). To test this approach I will monitor the self-assembly of a lipid bilayer and afterwards test the mechanical properties, more specifically the bending modulus.

Lipid bilayers are a very important biological structure due to it being the basis of almost all membranes in cells. The polar heads keep any polar or charged particles or molecules out thus making it a very effective structure and worth exploring with DPD. The chosen lipid 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) consist of a choline head group which is connected with the oleoyl and palmitoyl tails by a phosphate and glycerol group.

The simulation will be carried using the LAMMPS software which is a very flexible molecular dynamics simulator.

2 Methods

2.1 Dissipative particle dynamics

For DPD the idea is to find a force which follows the Langevin equation. The force on a particle i by other particles j is:

$$m\frac{\mathrm{d}v_i}{\mathrm{d}t} = \sum_{j\neq i} F_{ij}^C + F_{ij}^D + F_{ij}^R. \tag{1}$$

There are three different components to the force, namely the conservative force F^C, the dissipative Force F^D and the random force F^R. All forces depend on a weight function:

$$w(r_{ij}) = 1 - r_{ij}/r_c. \tag{2}$$

The conservative part is a simple linear repulsion with a constant which depends on the particle pair i, j:

2.2 Coarse-grained methods

The most important part of the CG models is the representation of different groups of atoms. In MARTINI there are five different basic bead types: water (W), polar (P), non-polar (N), a-polar (C), charged (Q). The P and C beads are also given a number from 1 to 5 depending on the polarity, reaching from P1 being the least polar and P5 being the most polar and C1 being the most a-polar and C5 the least a-polar. The W bead is identical to the P4 bead. The Q and N bead can also have subtypes which quantify the likeliness of hydrogen bond forming capabilities. There is 0 meaning no capabilities, d meaning some donor capabilities and a meaning some acceptor capabilities.

Applying this to the POPC lipid we have the Q0 choline head group, the Qa phosphate group, the two Na glycerol groups which connect to the two tails consisting of respectively 4 C1 or 3 C1 and 1 C3.