Multiscale methods for soft matter physics

Maurizio Gilioli

Contents

1 Definition of soft matter

2

Chapter 1

Definition of soft matter

Soft matter is plastic (polymers), water (liquids), air (gas), liquid crystals and colloidal suspensions (particles in liquid), gels, sand (granural materials). Also active matter (such as bacteria and fishes and birds are soft matters in some sense).

What is not soft matter: graphite is a dense matter, but grapheene is a soft matter. metals functionalized with proteions or nanoparticles could be considered as soft matter.

Poor definition:

Definition 1. Soft matter systems SM systems are deformable upon stresses of the order of magnitude of thermal fluctuations

This is an antropocentric definition! as in fact you are referring to our body termperature. Some elements become soft matter with the Temperature.

Soft matter is **mesoscopic**: RELEVANT STRUCTURES ARE MUCH LARGER THAN THE CONSTITUENTS BUT MUCH SMALLER THAN THE WHOLE —> you don't need very profound analysis to define and characterize your system. By coarse graining, you have to select space and time scales that are good for your system.

In general, you generate a coarse-grained system whenever you consider as indipendent compounds groups of atoms. The larger the size of the phenomena you are trying to observe, the less are the important details you have to consider!

The first level of approximation is done through the Born-Oppneheimer approximation, in fact through that method you can consider the electrons and the nuclei separately (at first by solving the so called the electronic problem, after by solving the motion of nuclei through Newton mechanics).

To go from a scale to another, you need a mapping function $\underline{R}_I = M(\underline{r})$. This determines

- loss of degrees of freedom (loss of information). in fact, several high resolution can produce the same low resolution arrangement.
- substantial increase of entropy in the system: you gain an effective entropy that you have to take into account, although you loose some simplifying.

Machine L. can be used to extract features useful for the coarse graining.