Introduction to Classical Molecular Dynamics

Dr. N. Faginas-Lago, Noelia
Dipartimento di Chimica, Biologia e Biotecnologie
noelia.faginaslago@unipg.it

The molecular dynamics describes the time evolution of molecular systems using classical mechanics. Molecular dynamics is, a computational method and its application represents a simulation of the system of interest. It is necessarily computational because an analytical solution for the dynamics of many interacting particles is mathematically impossible. Thus the solution offered by molecular dynamics is inevitably numerical in nature.

At heart molecular dynamics is an attempt to solve the classical equations of motion for a system composed of atoms and molecules with the aim of obtaining the time evolution of the system. The method is most often applied to condensed phase systems i.e. systems in the solid or liquid state, where the objective is to learn something about how the bulk properties of the system arise from the molecular basis. The time evolution aspect of molecular dynamics distinguishes it from the Monte Carlo method, in which the molecular system evolves through a stochastic or random-walk process rather than a true dynamical process.

This gives molecular dynamics a handle on time dependent properties, which means it is particularly useful for exploring transport properties, such as diffusion, thermal conductivity and viscosity, or aspects of spectroscopy, such as solvation induced spectral shifts, or the kinetics of chemical processes – all areas in which the dependence on time is the key factor.

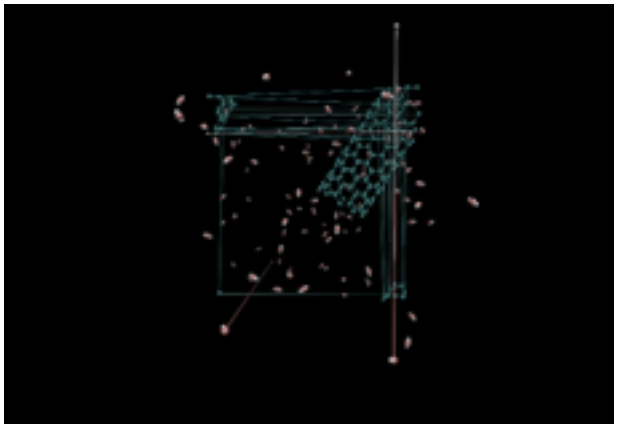

Illustration of the Periodic Boundary Conditions using DL_POLY package[1] for a SWCNT simulation.

[1]http://www.ccp5.ac.uk/DL_POLY/