basque center for applied mathematics

Molecular Modeling of Matter: What Can We Do Now, and in the Near Future?

Lecturers: Keith Gubbins[1] and Jesús M. Ugalde[2]

Date and time: 28 March – 1 April 2011, from 11:00 to 13:00.

Abstract: This course will provide an introduction to modeling at the electronic, atomistic and meso-scales of matter. Computational quantum mechanical methods, with some emphasis on density functional theory, will be discussed in the beginning of the course, followed by a more detailed treatment of molecular simulation methods (molecular dynamics and Monte Carlo) based on numerical solution of the equations of semi-classical statistical mechanics. The method of molecular dynamics (MD) will first be discussed, in which Newton's second law, force equals mass times acceleration, is solved for every particle in the system by finite difference methods. Since the dynamics of the particles is followed over time, it is possible to calculate transport and other dynamical properties in MD, in addition to equilibrium ones. Moreover, the particles move naturally under the influence of their inter-molecular forces, in contrast to MC. The Monte Carlo (MC) method, a stochastic method of generating a Markov chain of molecular configurations that are sampled according to the probability laws of statistical mechanics, will then be described. In Monte Carlo trial changes to the molecular configuration are accepted or rejected according to the probability laws, thus generating a chain of configurations that obey the equilibrium probability law; by averaging over this chain we can calculate the equilibrium properties of the system – thermodynamic functions, atomic structure of the material and other equilibrium functions. We will derive the acceptance criteria for several sets of independent variables – the canonical (N, V, T), grand canonical (μ, V, T), microcanonical (N, V, E) and isothermal-isobaric (N, P, T) variables, where N, V, T, μ, E and P are number of molecules, volume, temperature, chemical potential, energy and pressure. Finally some commonly used meso-scale methods will be described, in which the atomic structure of the material is coarse-grained, so that the material is regarded as made up of 'blobs' of matter. Such coarse graining enables much larger systems, and longer time scales, to be studied, at the cost of losing atomic detail and a rigorous basis for the calculations.

Programme:

Day 1. Introduction to atomistic simulation methods. Molecular dynamics simulation methods. Finite difference algorithms. Constraint molecular dynamics. [Prof. Gubbins]

Day 2. Semi-classical statistical mechanics. Canonical, Microcanonical and Grand Canonical ensembles. Monte Carlo method, Canonical ensemble. [Prof. Gubbins]

Day 3. Monte Carlo method in the Grand Canonical and Isobaric ensembles. [Prof. Gubbins]

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Day 4. Coarse graining and meso-scale methods. Lattice Monte Carlo. Brownian dynamics. Dissipative particle dynamics. [Prof. Gubbins]

Day 5. Quantum mechanical methods. Introduction, Hartree-Fock approximation, electron correlation, density functional theory. [Prof. Ugalde]

Bibliography:

[1] D. Frenkel, and B. Smit, *Understanding Molecular Simulation*, 2nd edition. Academic Press, San Diego 2002.

[2] C.G. Gray and K.E. Gubbins, *Theory of Molecular Fluids*. Clarendon Press, Oxford, 1984.

[3] A.R. Leach, *Molecular Modeling: Principles and Applications*, 2nd edition. Prentice Hall, 2001.

[4] T. Schlick, *Molecular Modeling and Simulation*. Springer-Verlag, New York, 2002.