Introduction to Numerical Simulations: From Materials Science to Biochemistry

Mauro BOERO
IPCMS
boero@ipcms.u-strasbg.fr

Numerical approaches have nowadays reached a stage where realistic simulations at the atomic-scale level of complex materials are possible. This is due both to improvements in the basic theory and to the remarkable development of last-generations computers. In academic and industrial laboratories, numerical simulations represent now a routinely used tool to perform virtual experiments suitable to complement the experimental outcome, to investigate materials at conditions not reproducible with present-day technologies and to predict materials properties or to perform chemical reactions in a cheaper way with respect to a mere experimental approach. The knowledge of the general principles of these approaches, their strength and also their limits can then be regarded as an important background for researchers working in the fields of materials science, chemistry and biology. The present course is aimed at providing a general introduction to the most advanced (and used) algorithms in numerical simulations to persons with a standard background in classical and quantum dynamics and thermodynamics. Theoretical approaches are presented and briefly discussed in their analytical form and in their numerical (discrete) version for computer coding. Examples of applications are given, providing an overview on the type of information one can extract and on the way these simulations can be designed to answer specific physical/chemical questions.

Main topics:

1. Classical Molecular Dynamics (MD):
   Newtonian and Lagrangean dynamics
   Basic algorithms
   Time averages and ensemble averages
2. First Principles MD:
   Brief review of DFT and Born-Oppenheimer approximation
   Car-Parrinello Molecular Dynamics (CPMD)
   Mermin functional and Free Energy MD (FEMD)
3. Hybrid schemes:
   Combined classical MD and DFT-based MD
4. Reactive schemes:
   General problem in chemical reactions
   path sampling methods
   Blue Moon ensemble approach
   Metadynamics

Time: Les cours auront lieu les 3, 7, 10, 14, 17, 21 décembre 2009 et les 5, 7, 12 et 14 janvier 2010 de 16:00 à 17:00 h.

Place: Salle 70
Institut de Physique et Chimie des Matériaux de Strasbourg
23, rue du Loess, 67034 Strasbourg

Contact : J.P. Bucher (03 88 10 70 96, bucher@ipcms.u-strasbg.fr)