Introduction to Numerical Simulations: From Materials Science to Biochemistry with a Look at Modern High Performance Computing Platforms

Mauro BOERO
IPCMS
mauro.boero@ipcms.unistra.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 high performance computers (HPC). In academic and industrial laboratories, numerical simulations represent nowadays a routinely used tool to perform virtual experiments suitable to complement the experiments, to investigate materials at conditions and/or atomic-level details not accessible in a laboratory by present-day technologies. This has disclosed an entire new field to predict materials properties or to perform chemical reactions in a cheaper way with respect to a mere experimental approach. The knowledge of the basic principles, 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 algorithms in numerical simulations to students with a standard background in classical and quantum dynamics and thermodynamics. Theoretical approaches are presented 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 from these numerical approaches.

1. Classical Molecular Dynamics (MD):
   Newtonian and Lagrangean dynamics: Basic algorithms
   Time averages and ensemble averages
2. First Principles MD:
   Brief review of Hartree-Fock approaches, Density Functional Theory and Born-Oppenheimer approximation
   First Principles Molecular Dynamics (FPMD)
   Mermin functional and Free Energy MD (FEMD)
   Practical Implementation on HPC architectures
3. Hybrid schemes:
   Combined classical MD and DFT-based MD: Hybrid QM/MM methods
4. Reactive schemes:
   General problem in chemical reactions
   Free Energy sampling techniques and reaction paths

Time: Les cours auront lieu les 9, 12, 16, décembre 2013 et les 10, 13, 16 janvier 2014 de 16:00 à 18:00 h. (12 heures)

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