Introduction to Numerical Simulations and High Performance Computing: From Materials Science to Biochemistry

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Advances in the theoretical methods and high-performance computing (HPC) platforms make nowadays numerical approaches a versatile, reliable and precise tool for performing virtual experiments, complementing the real ones, and providing access to details escaping experimental probes. This has paved the route to an entire new multidisciplinary field where design of materials with specifically tuned properties, advanced drug discovery or proteins and nucleic acids interactions represent just a few examples of the possibilities disclosed. Given this scenario, knowledge of the basic principles, their strength and also their limitations has become a fundamental 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 and methods in numerical simulations to students with a standard background in classical and/or quantum mechanics and thermodynamics. Theoretical approaches are presented and their analytical formulation discussed in view of their numerical (discrete) version required for any implementation in a computer code. Examples of applications are given, providing an insight into the type of information that can be extracted from these numerical approaches. Finally, an overview of the HPC architectures available to date and in the near future, along with their exploitation by parallel programming tools will be presented as a necessary complement to the basic theory developed for an efficient use of the continuously evolving technologies in massively parallel computing.

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 Hartree-Fock approaches and Density Functional Theory
   First Principles Molecular Dynamics (FPMD)
   Mermin functional and Free Energy MD (FEMD)
3. Hybrid schemes:
   Combined classical MD and DFT-based MD: Hybrid QM/MM methods
4. Advanced Methods: Reactive schemes
   Free Energy sampling techniques and reaction path sampling
5. Advanced Methods: Path Integral and non-Adiabatic Methods
   Quantum nuclei and surface hopping dynamics
6. Brief overview of parallel architectures and parallel programming

Time: Les cours auront lieu les 22, 24, 29, 31 janvier et 5, 7 février 2019 de 14:00 à 16:00 h. (12 heures)

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