DEPARTMENT OF MOLECULAR SCIENCE AND NANOSYSTEMS

Seminars of the PhD Programme in Chemistry

Multi-scale Modelling of Biological Systems Using Coarse-Grained and Hybrid Particle-Field Approaches

Michele Cascella

Department of Chemistry and Centre for Theoretical and Computational Chemistry (CTCC), University of Oslo, Norway

April 20th, 2017
at 15:00
Room D, 1° Floor Zeta Building

Abstract

Since the beginning of the informatics revolution, major e_ort has been put in developing reliable mathematical and physical computational models of complex systems at di_erent resolutions. In bottom-up approaches, the aim is to establish computational models based on fundamental physical principles that are able to predict the behaviour of the system of interest [1]. Even though atomistic simulations can now deal with systems as large as millions of atoms, and for simulation times reaching sometimes the millisecond, several biological processes involving large macromolecular complexes require description at time an sizes that go beyond even such di-mensionalities. In this seminar, I will present Coarse-Grained [2] and multi-scale computational strategies [3] aimed at reducing the intrinsic complexity in atomistic simulations. Such models make it possible to investigate systems composed by several hundred thousands to millions of atoms for several milliseconds on routinely available computational architectures. In particular, I will present recent advances [4] targeted at the study of polyelectrolyte multiphase systems like lipopolysaccharides, and in general complex bio-materials interface systems.

References

[1] M Cascella and S Vanni, in *Specialist Periodical Reports: Chemical Modelling* { Vol 12, 2015, pp. 1{52, RSC.

[2] M Cascella et al *J. Chem. Theory Comput.*, D Alemani et al *J. Chem. Theory Comput*. 2010, 6, 315; E Spiga et al. *J. Chem. Theory Comput*. 2013, 9, 3515. 2008, 4, 1378.

[3] G Milano et al *Phys. Biol*. 2013, 10, 045007.

[4] SL Bore et al in preparation, HB Kolli et al in preparation.

L'organizzatore
prof. Achille Giacometti

Il Vice-Coordinatore del Dottorato in Chimica
prof. Maurizio Selva

Università Ca'Foscari Venezia

dottorato.chimica