

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

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Since the beginning of the informatics revolution, major effort has been put in developing reliable mathematical and physical computational models of complex systems at different 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 and sizes that go beyond even such dimensionalities. 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

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