Computer simulations of soft matter: bridging the scales

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Abstract:

The definition of soft matter encompasses a wide variety of systems, ranging from simple liquids to biological macromolecules as well as artificial materials of great technological relevance. A unifying feature of these systems is the interplay of characteristic length and time scales, which determines their mechanical and dynamical properties. This multi-scale nature obviously represents a difficulty when it comes to simulations: in fact, the size of the system often makes it impossible to treat the whole of it at a fine-grained level.

In this talk I will give an overview of some of the computational strategies employed in our group to study soft matter. Examples include the topological entanglement of biomolecules, specifically proteins and DNA, and the techniques we developed to simulate molecular liquids. Particular emphasis will be given to adaptive resolution strategies, which allow the concurrent use of different models of the system at different levels of resolution.