



COLLOQUIA 2017-2018

Giovedì 8 Marzo 2018

Aula 102 "L. Giulotto", ore 16.00

Dipartimento di Fisica, via Bassi 6, Pavia

The devil is in the atomistic detail - Problems and solutions in computational soft matter

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Abstract: One of the most challenging aspects in the computational study of soft matter is its intrinsic multi-scale nature, that is, the fact that many relevant processes take place on a broad range of length and time scales. Their interplay often limits, and sometimes prevents, the usage of coarse-grained models, due to the lack of relevant chemical details. On the other hand, the large system sizes make it difficult if not impossible to employ a highly detailed yet computationally expensive atomistic representation. Dual resolution simulation methods aim at overcoming these limitations making use of different models with different resolution in a concurrent fashion, thereby employing a detailed description where strictly necessary, and an effective, coarse-grained model elsewhere. This seminar will provide an overview of the basic principles and techniques enabling this approach. Selected applications will be also presented, for cases of relevance in the field of biochemistry and protein science.