Position: Professor of Structure of Matter
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The focus of my research activity is on developing algorithms for Molecular Dynamics simulation of complex systems in condensed phases. From the from now ancient SHAKE algorithm (a procedure to introduce holonomic constraints in MD) or the Subtraction Technique (a noise reducing approach to compute the response to weak external fields in Nonequilibrium MD) to the introduction of the Blue Moon's ensemble (to simulate in MD rare events)and techniques to simulate Brownian motion to the most recent, and still very active, field of rigorous algorithms to compute nonadiabatic quantum-classical dynamics, the attempt is to widen the domain of computer simulation in condensed matter with a particular emphasis on MD (as distinguished from the very close but different MC- Monte Carlo). Together with that, I have been, and still am, also interested in challenging applications od atomistic MD simulations ranging from surface/interface physics problems in Materials sciences to simulations of biological molecules to find atomistic level explanations of their behavior or functioning mechanisms. More generally, I am interested in considering a variety of developments/applications in the simulation of systems of Statistical Mechanics interest.

Curriculum Vitae

Publications Updated 16 January 2015