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S E M I N A I R E

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" Further Perspectives for Holonomic Constraints in Molecular Dynamics "

Since more than sixty years Molecular Dynamics (MD) simulation (with its cousin Metropolis MonteCarlo) has provided the major tool to the progress of our knowledge of all non-trivial condensed matter systems (liquids, soft and biological matter, materials science, etc). A non trivial part in this remarked progress is due to the introduction of (holomic) constraints. At first holonomic constraints, once technically domesticated, permitted to extend MD from simple atomic to molecular systems, including large molecules (polymers, proteins etc). Then, once the ensemble of a system subjected to constraints was formally derived, the concept of a constrained system has been used, as a variety of Maxwell demon, to simulate rare events and, so, a variety of activated processes (the Blue Moon ensemble). During this evolution, the problem to represent by simulation both nonequilibrium situations and various thermodynamic ensembles, beyond the microcanonical one, has requested to extend the treatment of constraints to non-hamiltonian dynamics. Finally we have recently discovered that phantom zero-mass particles constrained to a system of real particles can be introduced to solve in a seamless manner the MD simulation of polarizable systems, still now a nightmare of MD practitioners. Further progress in this direction is in sight. The present seminar will review the results achieved and sketch some promising developments.

Vendredi 7 décembre 2018
11h00

Bibliothèque