Tuesday, November 6th, 16:00-17:00

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HOLONOMIC CONSTRAINTS AND STATISTICAL MECHANICS

In this talk we first review the state of the art of the numerical approach to a dynamical system submitted to holonomic constraints. Thus we define the way to conserve exactly the constraint conditions (by an algorithm universally known as SHAKE) and show how to integrate the equations of motion directly in the phase space of the natural Cartesian coordinates and momenta of the system. To do that we recall SHAKE and its numerical implementations in the notable cases of Verlet and velocity-Verlet algorithms. After discussing how constraints modify the properties of the equilibrium ensemble, we show how, thanks to Mark Tuckerman and Glen Martyna, at the price of moving to a dynamical system no more (directly) Hamiltonian, it is possible to provide a direct interpretation of the dynamical system and to derive its full Statistical Mechanics (both equilibrium and non-equilibrium). To achieve that, we generalize the statistical treatment to systems no longer conserving the phase space volume (equivalently, we introduce a non-Euclidean invariant measure in phase space) and derive a generalized Liouville equation describing the ensemble out of equilibrium (that includes the linear and nonlinear response theory of Kubo for systems subjected to constraints). We conclude with an observation opening to surprising applications.