



COLLOQUIUM DFA

Giovanni Ciccotti

Department of Physics
University of Roma "La Sapienza"

December, 17 - 3 PM
DEPARTMENT OF PHYSICS AND ASTRONOMY
Zoom meeting and YouTube streaming

The colloquium will be held in Italian

Molecular Dynamics, a new computational frontier of theoretical physics: from physical laws to reality

Computational power has developed at unbelievable speed. In a little more than 70 years the computing power has increased something like eighteen orders of magnitude, making possible the unprecedented technological revolution which characterizes our present times.

Not so known, instead, is the fact that this advancement has brought along a silent but deep change in the very foundations of Theoretical Physics, specifically to the part dealing with large aggregates of atoms and molecules – Statistical Mechanics and Molecular Simulation.

Molecular Simulation, i.e. the evolution and macroscopic behaviour of mathematical models of systems composed by a large numbers of molecules, born around the mid-fifties, is based on two new methods of mathematical physics, known as Molecular Dynamics and its close associate, Metropolis Monte Carlo. The gist of Molecular Dynamics is to show that the behaviour of aggregates of molecules be they in simple phases or complex polyatomic structures can be reconstructed/understood starting from the fundamental laws, without making use of intermediate/approximate theoretical constructions. At epistemological level, Molecular Dynamics can be seen as the realization of the dream of theoretical physicist: a direct route, applied to an increasing variety of physical, chemical and biological systems has been found, going directly from physical laws to the understanding and control of complex phenomena. The aim of this presentation is to introduce the new approach, explain its epistemological meaning and assess the nature of the transformation induced in theoretical physics.



Webinar zoom <https://indico.dfa.unipd.it/event/36/>
YouTube <https://www.youtube.com/c/AulaRostagniUnipadovaDFA>

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