Institute Lecture

Fluctuations and rare events

Professor Parrinello Michele

ETH Zurich, and
Università della Svizzera Italiana, Lugano, Switzerland

4th December 2017, Time: 6:15 PM, Venue: LH-17

Abstract

Computer simulations based on an atomistic description of matter have become one of the pillars of contemporary science. However in spite of their power, their scope is severely restricted by a variety of limitations that make their application to many complex systems challenging. One such limitation arises when the system exhibits long-lived metastable states separated by kinetic bottleneck. This is a common occurrence, for instance in chemical reactions, phase transitions, protein folding and in many other areas. The time scale for such rare but crucial events to occur, far exceeds what can be reached by direct simulation. We put in place a strategy for addressing this problem. We first identify the degrees of freedom that are involved in the process and then we amplify in a controlled way the fluctuations of these degrees of freedom such that the configuration space exploration is greatly accelerated and macroscopic time scales con be simulated. The role of entropy fluctuations is underlined. We use the example of crystal nucleation to illustrate these concepts.

About the speaker

Professor Michele Parrinello is currently Professor at ETH Zurich, and the Università della Svizzera italiana Lugano, Switzerland. He is known for his many technical innovations in the field of atomistic simulations and for a wealth of interdisciplinary applications ranging from materials science to chemistry and biology. For his work he has been awarded the 2011 Prix Benoist, the 2017 Dreyfus Prize and many others prizes and honorary degrees. He is a member of numerous academies and learned societies, including the National Academy of Science, the British Royal Society and the Italian Accademia Nazionale dei Lincei. He is the author of more than 600 papers and his work is highly cited.

Tea at 6.00 PM

All interested are welcome.

S. Ganesh
Dean of Research and Development, IIT Kanpur