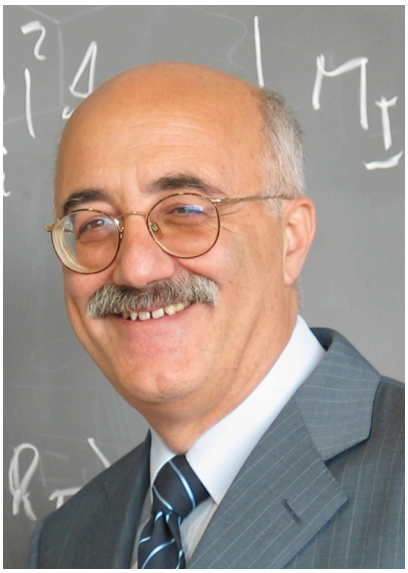
ACEnet Institute for Materials Modelling and Simulation
and Department of Physics and Physical Oceanography

AIMMS

Seminar

Michele Parrinello

Computational Science, Department of Chemistry and Applied Biosciences,
ETH Zurich, USI Campus, Via Giuseppe Buffi 13, CH-6900 Lugano,
Switzerland.



Friday, May 9th, 2008
3:30pm room C2045
coffee and doughnuts

Simulating Complexity: "Challenges and Progress in Atomistic Materials Science Simulations"

Computer simulation methods based on empirical potentials or on the *ab-initio* approach have made invaluable contributions to our understanding of complex chemical and biochemical processes. However in spite of great progress in hardware, computer simulations often fall short of what is needed for a realistic description of the systems of interest. It suffices here to mention the fields of nanoscience and biomaterials where systems composed of a large number of atoms need to be studied over very long time scales. In order to remedy this situation we are developing novel simulation methods that greatly extend the length and time scale of the simulation. We shall present a new approach to ab-initio molecular dynamics which accelerates simulations by at least one order of magnitude. In addition we shall describe methods for accelerating the study of slow processes and calculating free energies. These novel methods allow a wide class of difficult yet very important problems to be studied. We shall present a number of applications to structural phase transitions and nucleation. The application and further development of these methods promises to go a long way towards pushing further the limits of computer simulation.

Professor Parrinello 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. Together with Roberto Car he introduced ab-initio molecular dynamics, also known as the Car-Parrinello method, marking the beginning of a new era both in the area of electronic structure calculations and in molecular dynamics simulations. He is also known for the Parrinello-Rahman method, which allows crystalline phase transitions to be studied by molecular dynamics. More recently he has introduced metadynamics for the study of rare events and the calculation of free energies. For his work he has been awarded many prizes and honorary degrees. He is a member of numerous academies and learned societies, including the German Berlin-Brandenburgische Akademie der Wissenschaften, the British Royal Society and the Italian Accademia Nazionale dei Lincei, which is the major academy in his home country Italy. Born in Messina in 1945, he got his degree from the University of Bologna and is currently professor of Computational Sciences at ETH in Switzerland.