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Computational sciences: new opportunities

A new way of 'doing science' has recently joined the traditional theoretical and experimental disciplines. Computer-based numerical simulations are now replacing laboratory tests when the latter are unaffordable, or too hard to conduct or interpret. Computational sciences, which involve the use of increasingly faster and more powerful computers, enable the development of algorithms, models and software suitable for studying complex phenomena. Located on USI's Campus since 2001, Prof. Michele Parrinello's research group works on computer simulations of highly complex phenomena in physics and chemistry; the innovative computational methods it develops have acquired worldwide reputation. In addition, the team's research concentrates on various biology phenomena and the characteristics of some materials.

In a matter of years, technological progress has provided the means for computer performance to grow exponentially. Today, super-calculators (the so-called petaflops machines) can perform a high number of mathematical operations per second. The computational power of these new-generation machines allows them to solve highly complex problems which until some years ago had been considered insoluble by applying sophisticated modelling and numerical simulation methods.

Housed on USI's Lugano Campus since 2001, the research group in computational science of the Swiss Federal Institute of Technology, Zurich (ETHZ) applies the experimentation and numerical simulation methods of scientific computing to the study of physical and chemical phenomena of great complexity.

Prof. Michele Parrinello, who leads the research group, explains: *"Numerical simulation as a way of 'doing science' has emerged in the past few decades. There are different reasons for conducting simulations: practical, when they help us carry out experiments that could otherwise not be performed in a laboratory (too costly or too dangerous); or conceptual, when an experiment can measure some parameters but fails to show what happens to the system as a whole"*.

Computational sciences at USI

Computational sciences are a great opportunity for USI to tackle highly complex problems ranging from the exact and natural sciences to economics and the social sciences, including biomedicine, ecology, as well as materials and engineering. The foundation in September 2008 of the Institute of Computational Science (ICS) at the Faculty of Informatics-USI was intended to promote and coordinate teaching and research in topics where the study requires extra-powerful computational tools. The rationale behind ICS lies in the novelty and sustainability of the initiative, but no less on the proximity in the regional academic and scientific contexts of peer partners such as the Swiss National Supercomputing Centre (CSCS), the Institute for Research in Biomedicine (IRB), the Oncology Institute of Southern Switzerland (IOSI), the Department of Innovative Technologies-SUPSI and the computational science team of the Swiss Federal Institute of Technology, Zurich (ETHZ), resident on USI's Lugano Campus and headed by Prof. Parrinello.

The computational science research team, headed by Prof. Parrinello.

Prof. Parrinello is, with Prof. Roberto Car, the joint author of the Car-Parrinello method, which combines molecular dynamics simulations with electronic theories, in order to determine what happens to atoms when they move and react with each other. The method evolved over the years, becoming more refined, to the point that today it is applied to countless fields, such as physics, molecular biology, chemistry, and geology.

We can draw various benefits from the method based on molecular dynamics simulation. For example, it is applied to enhance the catalysis of chemical reactions, thereby reducing costs in the industrial production of plastic materials such as polyethylene or polypropylene. Or again, it helps forecast natural catastrophes (e.g. earthquakes), by analysing the behaviour of certain elements inside the earth, subjected to different levels of temperature and pressure.

There is nonetheless a limit arising from the costs of simulations: the size of the system (maximum number of atoms or molecules that can be processed) and the time scale (maximum duration of physical phenomena that can be simulated).

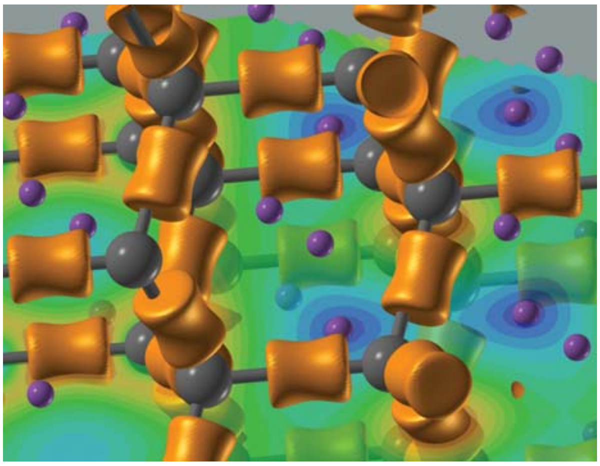
Areas of research: metadynamics and materials science

A research line pursued by the computational science group is the development of a method for the simulation of ever larger systems stretching over longer and longer periods, with a view to reaching increasingly precise calculations and obtaining ever more realistic results.

Prof. Parrinello explains: *"The main contribution of our research group in Lugano is a method called metadynamics, whereby we can simulate and observe long time scale phenomena. This method lowers the time barrier and serves in the study of some biological processes, for example protein misfolding, which results in neurodegenerative diseases such as Mad Cow (BSE), Parkinson's, or Alzheimer's diseases, and the interaction between enzyme and pharmacological drug"*.

On the enzyme-drug interaction, the research team led by Prof. Parrinello has joined forces with Prof. Ricardo A. Broglia (Faculty of Physics, State University of Milan) on a project aimed at inhibiting the folding of protease, an enzyme that is essential for the survival of the HIV virus. The virus can alter the amino acids of the protease very fast, reducing the affinity between enzyme and drug (in other words the drug's efficacy). So the objective is to prevent the folding of protease in the structure where this protein becomes active. This is how we facilitate the production of new drugs designed to block enzyme activity.

In addition, metadynamics has a major role in the study of the very complicated movements of some proteins: *"We are analysing a class of proteins known as Cox, connected with infectious processes, and hope to create specific drugs to target the proteins that generate the infection while preserving those that are useful. If that were possible, we could for example come up with an aspirin tablet that has no side effects"*, Parrinello exemplifies.



A snapshot of a light alloy made up of lithium and aluminium atoms.

Materials science is another important area of research. Here, the objective is the production of energy assuming a future where the economy is powered by hydrogen rather than hydrocarbon (fossil fuel). In this hypothetical scenario we would be allowed to exceed the limits imposed by the use of non renewable energy sources and to achieve an environmentally friendly, sustainable system of energy production. Hence the challenge is how to identify light materials for the storage of hydrogen. To this end, researchers are experimenting with light alloys (for instance a combination of lithium and aluminium atoms, see picture) to be used as containers or tanks to be easily tapped for hydrogen, without any excessive energy wastage.

Michele Parrinello (see picture) is currently professor of Computational Science at the Swiss Federal Institute of Technology, Zurich. He is renowned for his many technical innovations in the field of atomic simulations. Jointly with Roberto Car, in 1985 he formulated the *ab-initio* molecular dynamics method (known as Car-Parrinello Method), heralding the dawn of a new era not only for electronic structure calculus, but also for molecular dynamics simulations. He is also the co-inventor of the Parrinello-Rahman Method, used to explore the transition towards the crystalline phase by means of molecular dynamics. He has been awarded several prizes and distinctions for his achievements, and the membership of prestigious academies: the *Berlin-Brandenburgische Akademie der Wissenschaften*, the British Royal Society, and the Italian *Accademia Nazionale dei Lincei*.

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