Fact sheet

The development of computers, which can process enormous amounts of data incredibly quickly, has had a vast impact on all aspects of society. Science, in particular, has been transformed by this ability to quickly analyze data and has played an important role in driving their development. Furthermore, the new field of computational science has been developed based on computers and bridges the gap between scientific theories and the increasing complex experiments that are performed to test them. In computational science we take the equations that are known to govern the behaviour of the world and use them to formulate a highly accurate description of physical phenomena. In this way we can move out of the lab and instead perform numerical experiments using only a computer. This is useful because experiments are expensive, dangerous and in many cases downright impossible. There is thus no branch of science that has not been influenced by these numerical experiments, or as they are often called, simulations.

The development of modern computational science has been greatly influenced by the enormous increases in computational power that have happened over the last fifty or so years. However, the development of methodologies (algorithms) has had an equal, if not greater, influence. Professor Parrinello is known throughout the world for a number of widely used algorithms, many of which are named after him. In particular, he was involved in the development of the Parrinello-Rahman method, which is used to study crystalline phase transitions, and metadynamics, which can be used to accelerate simulations. Above all he is best known for the development of the Car-Parrinello method for *ab-initio* molecular dynamics, which has an enormous impact across a wide range of disciplines. As well as developing new methods Professor Parrinello has also applied these tools to a variety of systems in chemistry, biology, physics and biophysics.

In Professor Parrinello's simulations matter is described in terms of its most elementary components; namely the atoms, molecules and electrons. Hence, by combining the data produced by these simulations with the magic of modern graphical computers we can watch the motions of these basic components during a phase transition or chemical reaction. These simulations can therefore be thought of as providing a virtual microscope.

The methods developed by Professor Parrinello and their descendents have important, practical applications that can be useful to industry. For instance, the methods can be used to find useful new materials, to develop more efficient and less wasteful chemical processes, and to aid in the discovery of new drugs. Naturally these methods also have many applications to important problems that exist in a more academic setting. For example, they can be used to study materials at the high temperatures and high pressures at which they are found inside the earth or inside other planets, such as Jupiter or Neptune. Finally, we can also shed new light onto the strange properties of that most ubiquitous of materials, water, that are so essential for the origin of life.