Quantum and classical molecular dynamics

Research opportunities 2017-2018 *Prof Dmitry Shalashilin (d.shalashilin@leeds.ac.uk)*
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In 1929 Dirac stated that: "The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved." Only recently however, many years later, have atomistic simulation methods started to emerge that allow the treatment of quantum systems with many degrees of freedom, overcoming the difficulty noted by Dirac. Leeds Quantum and Classical Molecular Dynamics group develops new computational methods for atomistic simulations in chemistry and physics. These methods can treat bigger molecular systems faster and more accurately. They can visualise what happens at in atomic and molecular level.

There are two main research projects available. First project is focused on ***quantum dynamics*** in chemistry and physics. Chemistry is about rearranging nuclei whose motion is often quantum. Understanding tunnelling, zero point energy, quantization of vibrational and rotational motions and transitions between electronic states is crucial for chemical dynamics. We develop new techniques which speed up quantum simulations and allow to treat larger molecular systems[1-3]. The main idea is to use classical mechanics to guide quantum basis, which is illustrated on the figure below showing a trajectory guided grid following the wave function

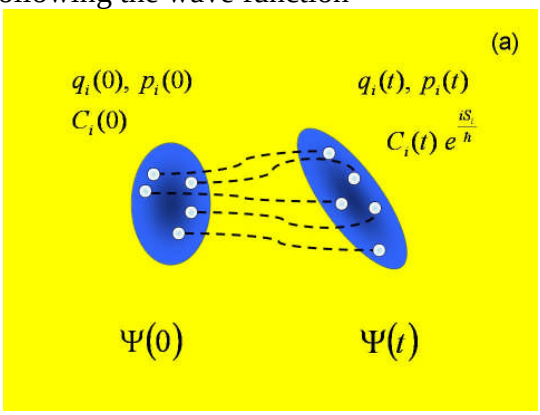

Figure 1. Quantum trajectories

We developed several methods, which exploit this very simple idea, and applied them to many interesting problems in chemistry and physics which range from chemical dynamics on ultrafast femtosecond time scale[4] to dynamics of electrons in laser field[5] and even quantum computers[6].

Second project is focused on ***classical Molecular Dynamics (MD) of biological molecules*** such as proteins and peptides. Classical MD disregards quantum effects but can treat realistic molecular systems comprised of thousands of atoms. The problem with classical molecular dynamics is that for molecules of this size atomistic simulations can be done on the time scale of picoseconds but the time scale of important biological processes such as protein folding for example is microseconds or longer so that at least 6 orders of magnitude has to be bridged. We developed efficient methods which allow to solve this problem by recovering long time dynamics from a set of short time simulations[7].

We apply our methods of accelerated classical MD to the investigation of protein unfolding[8], and peptide cyclization. For example with the help of our new methods we work on computational design of cyclic peptides[9], which currently are considered as prospective new antibiotics and anticancer drugs.

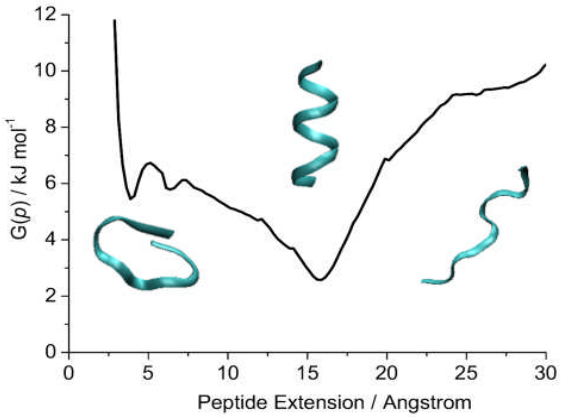

Figure 2 Peptide cyclization

Our research is very mathematical and involves the use of powerful computers. Both projects are suited not only for chemists but also for physics and mathematics graduates

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