Numerical methods for electronic structure calculation

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First-principle molecular simulation based on electronic structure calculation has become an essential tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. It is also an inexhaustible source of exciting mathematical and numerical problems.

In this talk, I will briefly introduce Density Functional Theory, which is to date the most widely used approach in electronic structure calculation, as it provides the best compromise between accuracy and computational efficiency. I will present some recent progress made in the mathematical understanding and the numerical analysis of this model, which pave the road to high-fidelity numerical simulations (with a posteriori error bounds) of the electronic structure of large molecular systems. I will then discuss the difficult issue of coupling the Kohn-Sham model with coarser models in view of simulating even larger molecular systems, such as drug-protein complexes in solution, or functionalized 2D-materials.

Numerical methods in molecular dynamics

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Molecular dynamics is now a very widely used tool to study by numerical simulations the matter at the molecular level. It is used in various fields, such as biology, chemistry or materials science in order to relate the macroscopic properties of matter to its atomistic features for various applications: protein structure prediction, drug design, dynamics of defects in crystals, exploration of the properties of new materials, etc...

Despite the increasing computational power, it remains in some practical cases difficult to simulate a sufficiently large number of atoms over sufficiently long timescales to obtain predictive and precise results. Mathematics play a fundamental role to derive coarse-grained models and to analyze and improve algorithms which are used to bridge space and time scales. One of the numerical difficulty is indeed related to timescales: the typical timescale of a molecular dynamics simulation is much smaller than the typical timescale at which the crucial events, from a macroscopic viewpoint, occur. This is related to the metastability of a molecular dynamics trajectory.

Many methods have been proposed in the molecular dynamics community to deal with these difficulties, and we will focus on two prototypical ones for which a mathematical analysis gives useful insights. We will first present adaptive importance sampling techniques, which have been proposed to sample efficiently statistical ensembles. Then, we will describe a mathematical analysis of accelerated dynamics methods which have been introduced by A.F. Voter to generate efficiently metastable dynamics.