PARTIAL DIFFERENTIAL EQUATIONS FOR MOLECULAR SIMULATION: A GUIDED TOUR

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ABSTRACT. Molecular simulation is one of the most vibrant field of scientific computing. It has a very broad scope of applications, ranging from chemistry and drug design to materials science and nanotechnologies. It is also a inexhaustible source of exciting mathematical and numerical problems of various nature [1, 2]: linear and nonlinear PDEs, optimization and control, stochastic processes and Monte Carlo methods...

In this lecture, I will first give examples of applications of molecular simulation in engineering, astronomy and life sciences. I will then review some of the PDEs encountered in the field. Some of them (e.g. the Poisson equation, the linear Schrödinger equation) have been widely studied by the applied mathematics community. Others would certainly desserve more attention. In particular, about 30,000 scientific papers published in 2018 contain numerical simulations of the Kohn-Sham model. This model is based on Density Functional Theory (DFT), for the development of which Walter Kohn was awarded the Nobel Prize in Chemistry in 1998. It can be formulated as a coupled system of nonlinear elliptic partial differential equations (more precisely of nonlinear elliptic eigenvalue problems). Yet, the Kohn-Sham model is only mentioned in a handful of textbooks and monographs on numerical methods for partial differential equations. I will finally give three examples of on-going multidisciplinary works involving applied mathematicians, physicists and chemists, illustrating the diversity of the numerical problems arising in molecular simulation [3, 4, 5, 6, 7, 8].

Keywords: Density Functional Theory, Kohn-Sham model, Poisson equation, Schrödinger equation, domain decomposition, error estimators, reduced models

Mathematics Subject Classifications (2010): 35Q40, 65M15, 81Q05

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