Data-Driven Computational Physical Chemistry using Machine Learning Force Field

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Since the early days of computational molecular mechanics, the field has kept pushing against the intrinsic limits of whatever simulation method was available at the time. The most direct way to push that boundary now comes from machine learning. A Machine Learning Force Field (MLFF), in its most naive description, is a function that takes atomic coordinates as input and returns the energy and the force on each atom, which is all you need to run a molecular simulation. Once trained on ab-initio calculation data, an MLFF gains two things at once: speed and accuracy. It can bring a system of thousands of atoms to tens of nanoseconds within a few days, and its accuracy stays almost on par with the ab-initio method it was trained on.

In this seminar, I will start by briefly introducing how an MLFF works, then move on to its performance together with its strengths and weaknesses. After that, I will walk through a few of my own studies on dielectric constants, aqueous solutions, and chemical reactions, showing how problems that were not within reach of conventional computational chemistry can now be approached with MLFF, and how our physical-chemical understanding of these systems can be pushed further in the process.