Polarizable versus non-polarizable interaction models in simulations of fluids

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Any molecular simulation is associated with two choices: (i) force field, i.e., an intermolecular interaction model with specified parameters and (ii) simulation methodology. The former choice depends on the goals of simulations and the latter with the former choice and also with the goals of the simulation study. Whereas in theoretical studies even very simplified model can be used, in studies of real systems aiming at prediction of their properties the best available models should be used. However, this has not been always the case for a number of reasons.

After decades of using rigid pairwise additive models, with advances of quantum chemistry and computer technology, along with sufficient amount of gathered experimental evidence, it is time that pairwise non-additive interactions be incorporated into interaction models used in simulations.
Incorporation of polarizability represent the most natural first step beyond pairwise additivity. However, it also brings a number of problems which seem to be the main obstacle for a wider application of polarizable models.

In the first part of the talk several examples will be given demonstrating incapability of pairwise additive models to capture, not even qualitatively, behavior of certain fluid systems and and then a recently developed new Monte Carlo method, the Multi-Particle-Move MC, will be discussed in detail along with its different implementations for specific goals. At the end of the talk ethic of publishing simulation data will be briefly mentioned.