Force Field Parameterization from a Force Matching–like Approach: Merits, Shortcomings and Future Perspectives.

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Among the various approaches used in force field development, in recent years, the *Force Matching Algorithm* and similar approaches have been extensively used [1, 2, 3, 4, 5, 6, 7]. The method is based on a least square fit of reference properties (forces, torques, energies etc.) obtained with ab initio Molecular Dynamics simulations of condensed phase systems. Its advantage with respect to conventional schemes, lies in that only physically accessible configurations are sampled, and that the number of reference data per configuration is large. The main shortcoming of the method derives from the "quality" of reference simulations might not be as good as high level quantum chemical calculations. In this talk I will show our recent findings on tayloring of the penalty function; we have found thar a proper choice of weighting functions yields force fields that faithfully reproduce most of the ab initio dynamical and statical properties. In addition, the algorithm is used to unravel the limits of most widespread functional forms for the force fields. In particular, using water as benchmark, the impact of damping dispersion forces and Coulomb interactions at short range is assessed against ab initio results. Finally, pros and cons of this approach with respect to others are discussed, with particular emphasis on future applications to heterogeneous condensed phase systems, and to coarse grained force fields.

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