Development and implementation of accurate polarizable potentials for water and ionic liquid simulations

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Steady increases in computing power have enabled longer classical molecular dynamics simulations. The same increase in computing power may be harnessed to provide the means to perform simulations with more accurate potentials. We have been one of the main developers of the Gaussian Electrostatic Model (GEM), a force field based on explicit reproduction of molecular electronic densities. Here I will present the details for the development and implementation of a novel density–based force field, its parametrization for water and ionic liquid (IL) simulations and the parametrization of AMOEBA for ionic liquids. The density–based force field, which we call GEM*, combines GEM capabilities with modified terms from the AMOEBA force field. In particular, the Coulomb and exchange–repulsion intermolecular interactions are efficiently calculated with GEM, while the polarization, dispersion and bonded terms are determined using AMOEBA components. This new force field has been implemented in a modified version of pmemd in the AMBER suite of programs. Initial simulations of a GEM* water model show good results for both energies and forces compared to QM reference calculations, as well as comparison to experimental bulk properties (density, heat of vaporization, etc). These results, as well as timings of GEM* compared with AMOEBA will be discussed. I will also present results on our parametrization and simulations of imidazolium–based ionic liquids in GEM* and AMOEBA. Results for bulk properties for dimethyl–imidazolium with three different anions show very good agreement with experiment. These are to our knowledge, the first multipolar and density–based polarizable force fields developed for ionic liquids.