A general linear scaling implementation for polarizable embedding methods

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Polarizable QM/MM methods are a powerful strategy to model the effects of the environment on the properties of molecules embedded in a matrix, such as a solvent or a biological system. From a computational point of view, embedding schemes require to compute the electrostatic interactions among the MM sites and between the MM and QM region. The former operation, if performed in a straightforward manner, scales with the square of the number of MM site and can easily become a formidable computational challenge for large systems such as biological macromolecules. The cost of an embedding scheme is further aggravated if distributed multipoles are used instead of point charges and, even more, if the embedding scheme includes mutual polarization. In the latter case, a linear system of equations has to be solved for each given QM density[1].

In order to extend the applicability of (polarizable) embedding schemes to large and very large systems, it is paramount to reduce the computational cost associated with the aforementioned operations. *Mutatis mutandis,* such operations can be always written as the computation of some electrostatic quantity, such as the electrostatic potential or its derivatives, or its contraction with the sources. The computation of electrostatic quantities can be performed with a computational cost that scales linearly with the number of sources if a fast summation technique is used[2].

In this contribution, I will present a completely general implementation of polarizable embedding schemes that achieves linear scaling in computational cost and memory requirements. The implementation relies on the Fast Multipole Method[3] (FMM) to compute the required electrostatic quantities and can handle sources, including polarizable ones, up to the quadrupole. Furthermore, the implementation can handle excluded or scaled interactions between MM sites, as well as damped Coulomb kernels for the polarization interactions. I will show some scaling and timings for the specific case of the AMOEBA force field[4], which treats the electrostatics in terms of distributed charges, dipoles and quadrupoles and polarization via induced dipoles. Nevertheless, the framework can be easily extended to any other polarizable scheme and can also be generalized to arbitrary order multipoles.

References

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