

[P9] NEEMP – Tool for parameterization of empirical charge calculation method EEM

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Partial atomic charges describe the distribution of electron density in a molecule, and therefore they provide clues regarding the chemical behaviour of molecules. Atomic charges are frequently used in molecular modelling applications and they have also become popular cheminformatics descriptors [1, 2]. Because of not corresponding to any physical quantity directly, the partial atomic charges cannot be measured experimentally. However, they can be computed. One way of their calculation involves quantum mechanics (QM), methods which make no further assumptions and which use only physical constants. The principal disadvantage of QM methods is their computational complexity which limits their practical use to small systems only. For biomacromolecules or for simulations involving real-time charge calculations QM methods are not applicable.

For this reason empirical, significantly faster methods were developed. A very successful and popular empirical charge calculation method is the Electronegativity Equalization Method (EEM) [3]. It can produce charges whose accuracy corresponds to a QM method but it does not work per se, it requires a training phase in which numerous parameters corresponding to the base QM method and type of molecule are obtained. This parametrization is the most challenging part of EEM [4].

We developed NEEMP, a software tool for EEM parameterization. Its design goals are speed, robustness and universality. It works for wide range of molecular types, from small peptides to huge proteins, it can further improve the training set to achieve optimal results so that it is able to calculate parameters with high correlation (above 0.9). It use robust numerical methods, and the implementation can fully utilize current multi-core machines. Aside from the parameterization, NEEMP can also be used for fast EEM charges calculation and cross-validation of EEM parameters.

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