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Recent developments in the VOTCA package for coarse-graining

CHRISTOPH JUNGHANS, Los Alamos National Lab — Coarse-graining is a systematic way of reducing the number of degrees of freedom used to represent a system of interest. The Versatile Object-oriented Toolkit for Coarse-graining Applications (VOTCA) provides a uniform interface to commonly used coarse-graining techniques such as iterative Boltzmann inversion, force-matching, and inverse Monte Carlo. Further, it provides a flexible modular platform for the further development of new coarse-graining techniques. Recently two new methods for coarse-graining have been added to the package and got tested on SPC/E water and methanol-water mixtures. We will discuss these results in comparison to earlier structure-based studies, but also talk about the development of non-structure-based model.

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