

Abstract Submitted  
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**Coarse-graining using the relative entropy and simplex-based optimization methods in VOTCA**<sup>1</sup> VICTOR RÜHLE, Department of Chemistry, University of Cambridge, Cambridge, MARA JOCHUM, KONSTANTIN KOSCHKE, MPI-P, Mainz, Germany, N.R. ALURU, Beckman Institute for Advanced Science and Technology, Univ. of Illinois at Urbana-Champaign, Urbana, IL, USA, KURT KREMER, MPI-P, Mainz, Germany, S.Y. MASHAYAK, Beckman Institute for Advanced Science and Technology, Univ. of Illinois at Urbana-Champaign, Urbana, IL, USA, CHRISTOPH JUNGHANS, Theory Division, LANL, Los Alamos, NM, USA — Coarse-grained (CG) simulations are an important tool to investigate systems on larger time and length scales. Several methods for systematic coarse-graining were developed, varying in complexity and the property of interest. Thus, the question arises which method best suits a specific class of system and desired application. The Versatile Object-oriented Toolkit for Coarse-graining Applications (VOTCA) provides a uniform platform for coarse-graining methods and allows for their direct comparison. We present recent advances of VOTCA, namely the implementation of the relative entropy method and downhill simplex optimization for coarse-graining. The methods are illustrated by coarse-graining SPC/E bulk water and a water-methanol mixture. Both CG models reproduce the pair distributions accurately.

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