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Kirkwood-Buff analysis of liquid mixtures in AdResS: Towards an open boundary simulation scheme DEBASHISH MUKHERJI, Max-Planck Institute for Polymer Research, NICO VAN DER VEGT, Center for Smart Interfaces, TU Darmstadt, KURT KREMER, Max-Planck Institute for Polymer Research, LUIGI DELLE SITE, Department of Mathematics, FU Berlin — Many biophysical processes in water are determined by interactions of cosolvents with the hydration shells of dissolved (bio)molecules. Computational approaches to study these systems are mostly limited to the closed boundary simulations. While closed boundaries are perfectly suitable in many cases, problems arise when concentration fluctuations are large, or intimately linked to the physical phenomenon. For example, in non-ideal mixtures of water/cosolvent and a biomolecule, the excess of water/cosolvent, close to a protein surface, leads to water/cosolvent depletion elsewhere. This complicates a comparison with experiments that are conducted under osmotic conditions. Therefore, we use Adaptive Resolution Simulation (AdResS) scheme, which describes a small sub-volume of a much larger system in atomistic detail, maintaining thermodynamic equilibrium with a surrounding coarse grained reservoir. We show that the Kirkwood-Buff integrals (KBI), which directly connect thermodynamic properties to the molecular distributions, can be efficiently calculated within the small open boundary all atom region and the coarse-grained reservoir maintains the correct particle fluctuations. Results will be presented for the methanol/water mixture and solvation of amino acids in urea/water mixture.

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