Solvation free energies of aqueous mixtures in a "truly" open boundary simulation DEBASHISH MUKHERJI, KURT KREMER, Max-Planck Institute for Polymer Research — (Bio)macromolecular solvation in water cosolvent mixtures are dictated by the preferential interaction of cosolvents with the proteins. The numerical studies in the field are limited to the closed boundary schemes, which, however, suffers from severe system size effects. More specifically, when the conformational transitions are intimately linked to the large concentration fluctuations, the excess of cosolvents near a protein lead to depletion elsewhere in a small-sized closed boundary setup. This disturbs solvent equilibrium within the bulk solution. Therefore, by combining the adaptive resolution scheme (AdResS) with a metropolis particle exchange criterion, we propose a "truly" open boundary method that heals the particle depletion in a closed boundary setup. In AdResS, an all-atom region, containing protein, is coupled to a coarse-grained (CG) reservoir. Particle exchange is performed in the CG region, which otherwise would be impossible in an all-atom setup of dense fluids. We calculate solvation free energies within the all-atom region using Kirkwood-Buff theory. Our method produces well converged solvation energies that are impossible in a brute force all-atom MD of small system sizes. We will discuss two cases of triglycine in aqueous urea and PNIPAm in aqueous methanol.

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