28h Coarse-Grained Potentials from Widom's Particle Insertion Method

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We derive coarse-grained effective pair potentials using Widom's particle insertion method. Coarse-graining removes uninteresting degrees of freedom enabling one to explore phenomena at length and time scales not accessible in simulations of the original (atomistic) system. As an example, we compute effective potentials up to the pair level for a binary mixture of Argon (solvent) and Krypton (solute) where the degrees of freedom of the solvent, Argon, are integrated out. Comparison of the pair correlation functions of the effective system with those found in the full system reveals that the structure at the pair level is well represented by the effective system. However, we observe increasing deviations in the pressure as the density of Krypton is increased. These latter deviations are attributed to the neglect of three- and higher multi-body interactions. Comparison of Widom's method with an alternative route via the potential of mean force shows that while there is general agreement, Widom's method performs better at low solvent densities but experiences (the known) sampling difficulties at higher densities.