

475a A Unified Methodological Framework for the Simulation of Non-Isothermal Ensembles

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A general framework has been developed for the simulation of non-isothermal statistical mechanical ensembles. This framework is intended to synthesize the formulation of advanced "multi-ensemble" Monte Carlo simulation methods such as multihistogram reweighting, replica-exchange methods, and expanded ensemble techniques so that they can be applied to different non-isothermal ensembles. Novel implementations of these methods are demonstrated with different ensembles including the microcanonical, isobaric-isoenthalpic, and isobaric-semigrand ensembles. In particular, it is shown that the use of multi-ensemble methods allows the efficient simulation of microcanonical density of states, entropies, vapor-liquid and solid-liquid equilibrium for both pure component and binary mixtures. Systems investigated range from Lennard-Jones fluids to polymeric materials. In these applications, comparisons are also presented that underline the advantages of the proposed multi-ensemble implementations over alternative methods used before.