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Thermodynamically Constrained Inverse Monte Carlo Determination of Effective Pair Interactions HENRY ASHBAUGH, Tulane University, LU YANG, Tulane, SHEKHAR GARDE, RPI, SANAT KUMAR, RPI, TULANE COLLABORATION, RPI COLLABORATION — Bridging length scales with molecular simulations requires the development of effective interactions in which degrees of freedom are integrated out to reduce computational expense. Such coarse graining strategies often lose critical thermodynamic information as molecular detail is washed out. Inverse Monte Carlo methods which focus on the reproduction of fluid structure, for example, typically have heats of vaporization and vapor pressures which are significantly greater than experiment. We propose a new method, Thermodynamically Constrained Inverse Monte Carlo (TCIMC), which systematically constrains empirical potential functions to reproduce known energetics and pressures while minimizing the difference between experimental and model pair correlations. We demonstrate the application of TCIMC to the recovery of model pair interactions for the Lennard Jones fluid. This method is subsequently extended to the development of united atom potentials for the alkanes from more complex all atom descriptions. The development of thermodynamically consistent coarse grained potentials for the modeling of polymers is discussed.

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