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Optimal Ensemble Monte Carlo Simulations: Application to dense Lennard-Jones fluids SIMON TREBST, ETH Zurich, MATTHIAS TROYER, ETH Zurich — Broad-histogram Monte Carlo simulations directly calculate the density of states of a (quantum) system by sampling broad energy ranges and thereby give access to thermodynamic properties. While flat-histogram methods suffer from a critical slowing down, we have shown that the simulation of an optimized ensemble substantially speeds up equilibration and can efficiently overcome the entropic barriers which cause the slowdown [1]. In this talk, we present recent applications of the optimal ensemble method to dense Lennard-Jones fluids and particle-solvent models. Based on measurements of the local diffusivity an optimal ensemble that maximizes round-trip rates in radial coordinates can be simulated and the potential of mean force can be determined to high precision. The optimized histogram of the radial random walk reveals clear signatures of the intermediate transitions between shells of the dense fluid. [1] S. Trebst, D. A. Huse, M. Troyer, Phys. Rev. E **70**, 046701 (2004)

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