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Hybrid Monte Carlo Method In Path Space PATRICK MALSOM, FRANK PINSKI, University of Cincinnati — We are interested in understanding the ways a collection of atoms are able to undergo conformational change, or change of state. In particular, we are studying atoms as they move under Brownian (overdamped Langevin) dynamics. In many cases, such transitions are blocked by an energy barrier and conformational changes become rare events when the thermal energy is small compared to the barrier height. Our technique attempts to sample these transition paths efficiently while preserving the sample's thermodynamic significance. Our approach is based on a Hybrid Monte Carlo scheme (Beskos *et al.*) that incorporates auxiliary variables. The relative probability of paths is computed using the Onsager-Machlup functional. This method correctly handles the fractal nature of the Brownian paths. We illustrate this method by investigating one of the low energy transitions in the 14-atom Lennard-Jones cluster. In addition, we will show preliminary results for the gas-to-liquid transition in a 2-dimensional Lennard-Jones system.

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