

Abstract Submitted
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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 (over-
damped 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 sam-
ple 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 com-
puted 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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