Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Hyperdynamics boost factor achievable with an ideal bias potential[1] CHEN HUANG, DANNY PEREZ, ARTHUR VOTER, Theoretical Division, T-1, Los Alamos National Laboratory — Hyperdynamics has been proven to be very promising for bridging the time scale gap between simulations and experiments. Much effort has been devoted to developing valid bias potentials, however the limiting performance of hyperdynamics is still unknown. In this work, a nearly "ideal" bias potential is designed to study the limiting performing of hyperdynamics. This bias potential is constructed based on the minimum energy pathways (MEP) of all the pathways out of the current state. We apply this MEP-based hyperdynamics (MEP-HD) to several metallic surface diffusion systems. By using proper parameters for constructing such "ideal" bias potential, both the Kramers recrossings and the branch ratios of different transitions can be reproduced. Since such MEP-based bias potential is directly built on reaction coordinates, in most cases it gives boost factors that are orders of magnitude larger than the best existing bias potentials. Such impressive performance of MEP-HD is believed to be very close to the limiting performance of hyperdynamics, and shows that further development of hyperdynamics could have a significant payoff.

[1]This work was supported by the United States Department of Energy (US DOE) Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

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Date submitted: 12 Nov 2013 Electronic form version 1.4