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Finding lowest saddle point QING LU, Department of Mechanical Engineering and Division of Materials Science and Engineering, Boston University, MINGHAI LI, Gustaf H. Carlson School of Chemsitry and Biochemistry, Clark University, AKIHIRO KUSHIMA, Department of Materials Science and Engineering, University of Pennsylvania, XI LIN, Department of Mechanical Engineering and Division of Materials Science and Engineering, Boston University — A history-penalized basin filling algorithm is presented in this work which identifies the lowest saddle point starting from any given initial state on any given potential energy hypersurface. The natural analogy of this algorithm is filling a barrel with water; by monitoring the location where leakage occurs one identifies the lowest opening on the wall of the barrel. The successful implementation of this algorithm relies on insightful choices of the penalty function, penalty function combination, and peak refinement. Several types of penalty functions are implemented to study two classical systems, the ad-cluster surface diffusion and supercooled binary Lennard-Jones liquid, and one quantum system of the topological soliton migration. The most efficient penalty function is found to be a triangle penalty function with uniform forces and large 3N+1-dimensional volume. The combination of penalty functions dramatically improves the computational efficiency. The lowest saddle point can be precisely located by the basin filling algorithm coupled with a few standard peak-refinement methods.

Qing Lu
Dept of Mechanical Engineering and Division of Material Science
and Engineering, Boston University

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