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Effects of penalty function type on the history-penalized metabasin escape algorithm for supercooled liquids RAVI HEUGLE, XI LIN, Boston University — The history-penalized metabasin escape algorithm provides an autonomous transition state pathway for a trapped system to escape from deep metastable energy minima and larger basins of attraction. The effects of penalty function type on the efficiency of the algorithm are demonstrated by sampling portions of the potential energy surface of a binary Lennard-Jones liquid close to the glass transition temperature. Our results indicate that optimal penalty functions prefer both large 3N+1 dimensional volumes and the ability to force the system over a large range. The Gaussian, which until now has served as the standard penalty function used for activation, serves as the benchmark against other representative penalty function types. Analysis shows that the triangle function results in four fold improvements in efficiency over the Gaussian, thereby furthering the reach of simulation into timescale regimes largely inaccessible to molecular dynamics.

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