

Abstract Submitted
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Sampling saddle points on the free energy surface AMIT SAMANTA, Princeton Univ — We develop an algorithm for finding the saddle points on the free energy surface “on-the-fly” without having to find the free energy function itself. This is done by using the general strategy of the heterogeneous multi-scale method, applying a macro-scale solver, here the gentlest ascent dynamics algorithm, with the needed force and Hessian values computed on-the-fly using a micro-scale model such as molecular dynamics. The algorithm is capable of dealing with problems involving many coarse-grained variables. The utility of the algorithm is illustrated by studying the saddle points associated with (a) the isomerization transition of the alanine dipeptide using two coarse-grained variables, specifically the Ramachandran dihedral angles, and (b) the beta-hairpin structure of the alanine decamer using twenty coarse-grained variables, specifically the full set of Ramachandran angle pairs associated with each residue.

Amit Samanta
Princeton Univ

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