Abstract Submitted
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Acclerated rare event sampling DAVID YEVICK, University of Waterloo — We suggest a strategy for biased transition matrix Monte-Carlo calculations that both ensures the most rapid coverage of the entire computational window in the macroscopic variables of interest $\vec{E}$ and yields estimates of transition probabilities between states that are equally accurate in low and high probability regions. Further, paths between different low probability regions are sampled at regular intervals. For the case of a single E variable, a random system realization for which the value of E falls in e.g. the i:th histogram bin is generated. This state is perturbed and the resulting realization is rejected until a transition is observed to a neighboring bin, taken here as $i+1$. All accepted and rejected transitions are simultaneously employed to generate the elements of a transition matrix. Subsequently, only a transition to bin $i+2$ is accepted and this procedure is continued until the last of the N bins comprising the computational window is sampled. The procedure is then repeated but in the direction of decreasing bin number. The probability distribution of E can then be obtained by e.g. repeatedly multiplying a random vector by the transition matrix.

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