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Optimally efficient coarse-grained Monte Carlo simulation of rare transition events BABAK SADIGH, TOMAS OPPELSTRUP, Lawrence Livermore National Laboratory, WEI CAI, Dept of Mechanical Engineering, Stanford University, MAURICE DE KONING, MALVIN KALOS, VASILY BUOLATOV, Lawrence Livermore National Laboratory — We use the idea of coarse graining the multidimensional free energy landscape and present a new Monte Carlo scheme that allows for the exact calculation of the rate of rare transition events within the coarse-grained space defined by a few collective coordinates. This approach is based on a variational algorithm for determining an optimal importance function by which the absolute probability of sampling successful transition events is significantly enhanced, while the relative probabilities of any pair of successful events are preserved.

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