

Abstract Submitted
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How long does it take to measure eternity? Solving problems in hours that would take brute-force simulations the age of the universe¹
DAVID ADAMS, LEONARD SANDER, Department of Physics, University of Michigan, Ann Arbor MI, ROBERT ZIFF, Department of Chemical Engineering, University of Michigan, Ann Arbor MI — We present two new rare event techniques that we use to determine transition times in stochastic systems. We call the first technique forward flux sampling in time (FFST). This algorithm is similar to forward flux sampling (FFS) but doesn't suffer from the main flaw of FFS: a choice between either a slow initial flux calculation or an approximate solution for the transition time. The second algorithm, called the barrier method, is significantly more efficient than FFS and FFST, especially for transitions with long-lived meta-stable states. These algorithms can be applied to any problem that can be written as a Markov (memory-free) process. The barrier method is useful in relatively low dimensional problems. We present results comparing these new algorithms with FFS on 1D exactly solvable systems.

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