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Rare-event simulation methods for equilibrium and non-equilibrium events

ROBERT ZIFF, University of Michigan

Rare events are those that occur with a very low probability in experiment, or are common but difficult to sample using standard computer simulation techniques. Such processes require advanced methods in order to obtain useful results in reasonable amounts of computer time. We discuss some of those techniques here, including the "barrier" method, splitting methods, and a Forward-Flux Sampling in Time (FFST) algorithm, and apply them to measure the nucleation times of the first-order transition in the Ziff-Gulari-Barshad model of surface catalysis, including nucleation in finite equilibrium states, which are measured to occur with probabilities as low as 10ˆ(-40). We also study the transitions in the Maier-Stein model of chemical kinetics, and use the methods to find the harmonic measure in percolation and Diffusion-Limited Aggregation (DLA) clusters. co-authors: David Adams, Google, and Leonard Sander, University of Michigan. References: D. A. Adams, R. M. Ziff, and L. M. Sander, Computation of nucleation at a nonequilibrium first-order phase transition using a rare-event algorithm, Journal of Chemical Physics, 133, 174107 (2010) D. A. Adams, L. M. Sander and R. M. Ziff, The barrier method: A technique for calculating very long transition times, Journal of Chemical Physics 133, 124103 (2010) D. A. Adams, Yen Ting Lin, L. M. Sander and R. M. Ziff, "Harmonic measure for critical Potts clusters," Physical Review E 80, 031141 (2009)