

Abstract Submitted  
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**A rigorous approach to nonequilibrium Monte Carlo simulations**

ARIEL BALTER, Indiana University — Methods exist for mapping Monte Carlo time to real time in kinetic simulations, but these are not rigorously self-consistent because they are based on Boltzmann transition probabilities, which do not apply out of equilibrium. I present a rigorous method in which both transition probabilities and the time scale are self-consistently specified for any energy-based kinetic Monte Carlo simulation. I propose a method in which transition probabilities are still derived from an energy function, but not based on Boltzmann statistics. Although appropriate for nonequilibrium systems, this method recaptures detailed balance and Boltzmann statistics in the equilibrium limit.

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