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Mathematics Colloquium

Monday, November 11, 2019
Time: 4:00 p.m.
Location: Weber 223

Title: Efficient Simulation of Non-Equilibrium Systems

Abstract:

In statistical physics, the word \emph{non-equilibrium} is associated with irreversible processes, external driving forces, and dynamical quantities like rates of chemical reactions. Simulation of non-equilibrium systems is of fundamental importance in chemistry and biology. For example, non-equilibrium simulations have been instrumental in the interpretation single-molecule experiments. However, non-equilibrium phenomena pose special challenges for computation, especially when rare events are involved. We analyze a variant of Non-Equilibrium Umbrella Sampling (NEUS), a promising algorithm for the efficient simulation of non-equilibrium phenomena. We show that NEUS can be interpreted as a stochastic approximation procedure similar to the Robbins-Monro algorithm, and we present some results demonstrating its convergence and efficiency.

Host: David Aristoff

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