Dijkstra-like Methods for the Study of Rare Events

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ABSTRACT

Small-scale processes in physics and chemistry such as conformal changes in molecules are often modeled using stochastic differential equations with deterministic potential force and small noise. The events of interest are rare transitions between the metastable states of the system. I will discuss two approaches for the study of rare events whose important building blocks are the Dijkstra algorithm or Dijkstra-like solvers for Hamilton-Jacobi equations. The first approach is a finite temperature approach for estimating reactive flux through different reactive channels based on the analogy with electric networks. The second approach is a zero temperature approach for finding the asymptotic zero-temperature path and calculating the hierarchy of Freidlin’s cycles.