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Yuan Gao* (gao662@purdue.edu), 150 N. University Street, Math 736, West Lafayette, IN 47907. *Reversibility, stochastic optimal control and transition path simulation.*

Conformational transitions are very important in biochemical reactions. We reinterpret the transition paths theory from the stochastic optimal control viewpoint, which realizes the transitions almost surely. Based on collected high dimensional point clouds and nonlinear dimension reduction, we construct an approximated Voronoi tessellation for the reduced manifold and use it to construct an optimally controlled random walk on point clouds. To compute the mean transition path efficiently, a local averaging algorithm based on the optimally controlled random walk is developed, which adapts the finite temperature string method to the controlled Monte Carlo samples. (Received September 16, 2021)