

Continuous random walks (CRWs) are a powerful tool to model stochastic processes, which are ubiquitous in chemistry, biology, and physics. Since particles/molecules are often subject to both deterministic forces (electronic/magnetic/gravitational), as well as stochastic forces (Brownian motion, thermal fluctuations).

CRW are the mathematical equipment to model the time evolution of system dynamics to generate trajectories ensembles. Which are used to understand the system behavior, determine statistical properties, as well as analyze interesting processes such as rare events.

Rare events are vital to understanding of various physical phenomena because they generally constitute an important change that can precipitate a fundamental shift in the structure and properties of entire systems. The difficulty in studying this phenomena is due to the fact that they are rare and therefore extremely computationally expensive to simulate. The aim of this thesis to ameliorate the computational demand by examining a conditioned processes, which is achieved by constructing a Brownian Bridge. A Brownian bridge allows the simulation of a physical system where the event desired always occurs; therefore, allowing one to generate an ensemble of rare event easily and without expending excess computations on unimportant dynamics.

A key problem with the construction of a Brownian bridge is that it requires the solution to the Backward Fokker-Planck (BFP) equation, a partial differential equation (PDE) which suffers from the so-called curse of dimensionality, so obtaining its solution for high-dimensional systems becomes infeasible. To combat this, we search for methods to accurately approximate the correct solution with a substantial decrease in the computational cost. In one instance, we do this for barrier crossing problems, in which we use asymptotic methods to derive an analytical solution to the BFP for low noise systems, or at least one large energy barrier. In conjunction with importance sampling we show that this method accurately captures the conditional statistics for barrier crossing events. In another instance we examine paths at the tail end of the first passage time distribution, i.e. paths which stay within a region of phase space far longer than their mean escape time. We do this by utilizing linear operator methods to reformulate the BFP into a self-adjoint problem allowing the use of the spectral theorem. Along with the long-time approximation we show that this reduces the problem from a full PDE into only needing to solve for its dominant eigenfunction obtain an accurate bridge approximation.

When using a Brownian Bridge the drift of the conditioned process becomes singular near the endpoints. In the case of a rank-deficient diffusion tensor, the drift becomes more strongly singular which exacerbates the issue. To combat the numerical instabilities induced by the singularity, we can reformulate the bridge into a control-type problem. The purpose of which is to take advantage of the many powerful tools available in the field of stochastic optimal control. We employ this method to control the topology of semi-flexible polymer chains, whose governing SDE is rank-deficient. We replace the biasing drift term produced by the hitting probability with a control, then solving for the optimal controller becomes a minimization problem.