A Geometrical Method for the Smoluchowski Equation on the Sphere

Authors : Adriano Valdes-Gomez, Francisco Javier Sevilla

Abstract : We devise a numerical algorithm to simulate the diffusion of a Brownian particle restricted to the surface of a three-dimensional sphere when the particle is under the effects of an external potential that is coupled linearly. It is obtained using elementary geometry, yet, it converges, in the weak sense, to the solutions to the Smoluchowski equation. Rotations on the sphere, which are the analogs of linear displacements in euclidean spaces, are calculated using algebraic operations and then by a proper scaling, which makes the algorithm efficient and quite simple, especially to what may be the short-time propagator approach. Our findings prove that the global effects of curvature are taken into account in both dynamic and stationary processes, and it is not restricted to work in configuration space, neither restricted to the overdamped limit. We have generalized it successfully to simulate the Kramers or the Ornstein-Uhlenbeck process, where it is necessary to work directly in phase space, and it may be adapted to other two dimensional surfaces with non-constant curvature.

Keywords : diffusion on the sphere, Fokker-Planck equation on the sphere, non equilibrium processes on the sphere, numerical methods for diffusion on the sphere

Conference Title : ICCPM 2020 : International Conference on Computational Physics and Methods

Conference Location : Vancouver, Canada

Conference Dates : September 23-24, 2020