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SUPERSYMMETRIC LANGEVIN DYNAMICS TO FIND REACTION PATHS

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The dynamics of complex systems is often driven by rare but important events [1]. Well-known examples include chemical reactions, diffusion in solids and nucleation in phase transitions. The origin of the rare-event problem typically lies in the disparity between the thermal energy scale and typical energy barriers of the systems. In such a situation the dynamics of the system consists of a series of paths that remain in the vicinity of the metastable states for very long periods of time, followed by rare jumps from one state to another. We are interested in finding the paths that connect the metastable states (reaction pathways), as well as the associated transition rates. Many sophisticated techniques for this purpose have been developed over the past few years. Transition Path Sampling (TPS)[2], for instance, enables one to find transition mechanisms and rates, as long as the initial and final metastable states are known. Another recent technique to obtain the minimum energy path between two metastable states involves sampling the configuration space using strings , i.e., smooth curves involving an energy-based parametrization[3]. However, this method also requires prior knowledge of the states between which the transition occurs. Furthermore, both techniques require an initial path guess which, in principle, may exclude certain transition paths from the sampling.

We present a family of algoritmhs proposed in recent years [4] that allows one to find reaction pathways without prior knowledge of the final state or the requirement of specifying an initial path. The method is based on an analogy between the formalism of the Fokker Planck equation and supersymmetric quantum mechanics. This leads to a modified Fokker planck equation that allows one to obtain the reaction currents between metastable states of the system of interest. In practice, the approach is exploited using Langevin stochastic dynamics modified to get the reaction paths. Here we present some simple example toy models to show how this occurs.

The method is based on a Langevin dynamics with many walkers subjected to a branching or bias step in which the walkers are cloned or killed depending on an internal degree of freedom, which is the direction of the vector of the current reaction. Figure 1 shows the evolution of an initial group of walkers initially placed in one of the two metastable states of a bidimensional energy landscape. The Langevin dynamics then evolves the collection of walkers toward a stationary state in which the saddle points separating the metastable states becomes populated.

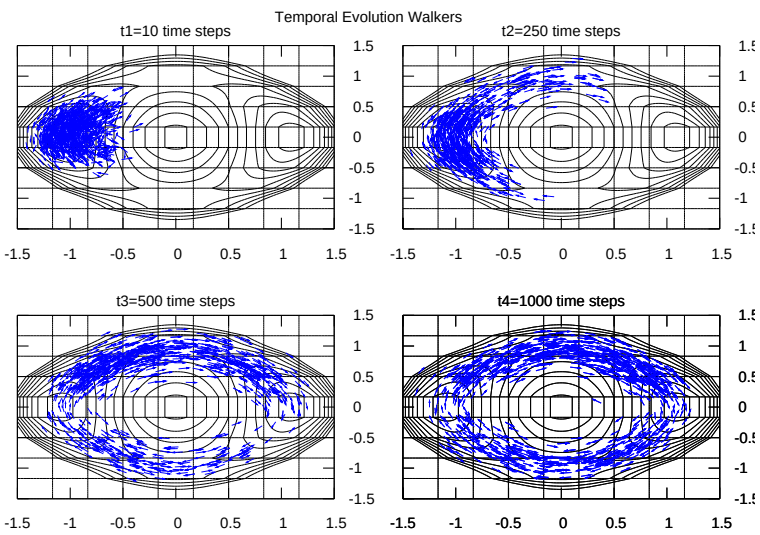

Figure 1 – Temporal evolution reaction paths, in a bidimensional energy landscape

The application of the approach looks very promising because it allows us to explore systems with large numbers of degrees of freedom without the need for specifying initial and final metastable states. As a result, the supersymmetric Langevin dynamics method permits a natural exploration of unknown metastable states as well as reaction mechanisms.

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