Enhanced sampling of dynamical trajectories, with and without machine learning

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The microscopic dynamics of many condensed matter systems occurring in nature and technology is dominated by rare but important barrier crossing events. Examples of such processes include nucleation at first order phase transitions, chemical reactions and conformational changes of biopolymers. The resulting wide ranges of time scales are a challenge for molecular simulation and numerous simulation techniques have been developed to address this problem. In the method of transition path sampling this is done by carrying out a Markov chain Monte Carlo simulation in the space of reactive trajectories. However, like other sequential sampling methods, TPS can suffer from statistical correlations, which reduce the sampling efficiency particularly in systems with multiple reaction channels. Here, I will discuss recent approaches, based on machine learning and on extending the sampling space, to reduce correlations in TPS simulations and provide insights into the kinetics and mechanisms of rare events.