The String Method for Saddle Point Search

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The dynamics of complex systems is often driven by rare but important events. Well known examples include nucleation events during phase transitions, conformational changes in macromolecules, and dislocation dynamics in crystalline solids. The main object of interest in these problems is the saddle points of the potential or free energy of the system. These saddle points act as bottlenecks (transition states) for the barrier-crossing event. In this talk, we show how the string method, which was originally proposed to compute minimum energy paths between two given states, can be used to compute saddle points for a given minimum of the potential or free energy. Application to the wetting transition on patterned surfaces will be presented.