Extension of the string method for saddle points search

Weiqing Ren, National University of Singapore and IHPC

The string method was originally designed for finding minimum energy paths between two minima of a potential (or free) energy. It evolves a continuous curve in the path space by steepest descent dynamics. In this talk, we discuss how the string method can be modified for saddle point search. Compared to the existing algorithms, the new method has the advantage that the computed saddle points are guaranteed to be directly connected to the minima. We will also discuss how the convergence can be accelerated using an inexact Newton method. This is a joint work with Eric Vanden-Eijnden.