Recent Development of Numerical Methods on Finding Saddle Point and Minimum Energy Path

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The dynamics of complex systems is often driven by multiscale, rare but important events. Finding saddle point and minimum energy path on an energy surface has attracted much attention in various areas such as nucleation in phase transition, chemical reaction, biology, etc. In this talk, I will present some recent progress on two different numerical algorithms:

1) Optimization-based shrinking dimer method, which reformulates the classical dimer method under an optimization framework. We then apply the Barilai-Borwein gradient method to achieve superlinear convergence;

2) Adaptive step-size string method, which treat the original string method as an iteration process to minimize the Friedlin-Wentzell functional.

We demonstrate that the Friedlin-Wentzell action can reveal how far from a general path to an MEP so that we can prove the adaptive step-size string method locally converges to the MEP.