数学与系统科学研究院

计算数学所学术报告

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报告题目：

Finite-temperature dimer method for finding saddle points on free energy surfaces

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上午 **11:00-12:00**

报告地点： 科技综合楼三层

311 报告厅

Abstract：

The dimer method and its variants have been shown to be efficient for finding saddle points on potential surfaces. When finite temperature effect is important for a high dimensional system, one usually need to describe the dynamics in a low dimensional space of reaction coordinates. In this case, transition states are collected as saddle points on the free energy surface. The traditional dimer method cannot be directly employed to find saddle points on a free energy surface since the surface is not known a priori. Here we develop a finite-temperature dimer method for searching saddle points on free energy surface. In this method, a constrained rotation dynamics of the dimer system is used to sample dimer directions and an efficient average method is used to obtain a good approximation of the most unstable direction. This approximated direction is then used in reversing the force component and evolving the dimer towards saddle points. Our numerical results suggest that the new method is efficient in finding saddle points on free energy surfaces.

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