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:

The String Method for the Study of Rare Event

邀请人: 季霞 副教授

<u>报告时间</u>: 2015 年 12 月 22 日(周二) 下午 16:00~17:00

<u>报告地点</u>: 科技综合楼三层 301 小报告厅

Abstract:

The dynamics of complex systems is often driven by rare but important events. Well known examples include nucleation events during phase transitions, conformational changes of macromolecules, and dislocation dynamics in crystalline solids etc. In this talk, I will present the string method for the study of such rare event. The string method finds the minimum energy path by evolving a curve, which is parameterized by its intrinsic arc-length, in the path space by steepest descent dynamics. I also show how the string method can be used to search saddle points (i.e. transition states) around a given minimum on potential or free energy surfaces. In the last part of the talk, I will discuss the extension of the string method to the space of collective variables.

欢迎大家参加!