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：

Mathematical Study of Milestoning

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上午 **10:30-11:30**

报告地点：　　科技综合楼三层 **311**

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Abstract:

Milestoning is a coarse-graining strategy that can serve both as an analysis tool to analyze time series of complicated activated processes and as a computational tool to accelerate the computation of these processes. It can be used, e.g., in the context of molecular dynamics simulations. In this talk, a solid mathematical foundation of milestoning is presented. For systems displaying metastability, the assumption of Markovian milestoning can be justified asymptotically provided that the metastable states are taken as milestones. Practically, the set of the metastable states can be identified automatically as the set that minimizes a metastability index, and a continuous-time Markov jump process can be built on this set by applying maximum likelihood estimation and Bayesian sampling techniques. For systems without the timescale separation, the assumption of optimal milestoning can still be justified for the set of milestones made of the forward isocommittor surfaces, which allows us to build a discrete-time Markov chain on the index set of milestones. For diffusion processes, under mild assumptions, by using a set of milestones made of the backward isocommittor surfaces, the mean first passage times between these milestones can be calculated exactly. In practice, the isocommittor surfaces can be identified approximately as the hyperplanes in the reaction tube by using the string method, and an accelerated sampling procedure based on the confined simulations in Voronoi cells can compute the required key objects in milestoning efficiently without the need to reinitialize simulations on milestones.

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