

Aspects of metastability in molecular simulation

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11 February 2026, 16:15 – 17:15* Berlin time
IRTG 2544: "Stochastic Analysis in Interaction"
— Berlin Probability Colloquium —

WIAS Berlin
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Abstract

The objective of this talk will be to present an approach we developed over the past 10 years to analyze metastable stochastic processes using quasi-stationary distributions. The interest of this approach is that it can be used to make a rigorous link between Markov processes with values in a continuous state space, and Markov processes with values in a discrete state space (i.e. the indices of the metastable states).

This is motivated by questions from molecular simulation, in particular to justify models based on jump Markov processes between states (kinetic Monte Carlo models) and to analyze related sampling algorithms (accelerated dynamics).

*Punctual, i.e. sine tempore!