Optimal Control of Complex Molecular Processes: A Mathematical Challenge

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Abstract: Molecular conformations are essential for the function of biomolecular systems. In terms of molecular dynamics conformations are metastable sets, i.e., the dynamics is trapped for long periods of time within a conformation and transitions between conformations are rare events. In the last decade mathematical approaches to conformation dynamics have achieved a lot of attention and have developed into standard tools in molecular research under the name "Markov State Models" (MSMs). This talk will outline the mathematical background of MSMs and present examples of real-world applications in drug design and protein folding. But the talk will also address the remaining fundamental problems in MSM building: Some transitions between conformations are extremely rare such that molecular dynamics simulations on the associated timescales are still infeasible, even on the largest computers. The second part of the talk will present how to overcome this obstacle by using ideas from optimal control of molecular dynamics.

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