

# Optimal control of molecular dynamics

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Molecular systems exhibits complicated dynamical behavior that is responsible for its (biological or nanotechnological) functionality. The effective dynamics can be characterized by the switching behavior between several metastable states, the so-called conformations of the system. Therefore, steering a molecular system from one conformation into another one means controlling its functionality. This talk considers (1) the construction of low-dimensional, so-called Markov state models (MSM) that describe the conformation dynamics of the molecular system, (2) new methods for efficient sampling of the rare transitions between conformations and (3) optimal control problems that appear relevant in molecular dynamics (MD) applications and their efficient solutions via MSMs.

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