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Dimensional Reduction of Markov State Models from Renormalization Group Theory

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Renormalization Group (RG) theory provides the theoretical framework to define Effective Theories, i.e. systematic low-resolution approximations of arbitrary microscopic models. Markov State Models (MSMs) can be shown to be rigorous Effective Theories for Molecular Dynamics (MD). Based on this fact, we use Real Space RG to vary the resolution of a MSM and define an algorithm for clustering microstates into macrostates. The result is a lower dimensional stochastic model which, by construction, provides the optimal coarse-grained Markovian representation of the system's relaxation kinetics. To illustrate and validate our theory, we analyze a number of test systems of increasing complexity, ranging from synthetic toy models to two realistic applications, built form all-atom MD simulations.

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