KINETICALLY CONSISTENT COARSE GRAINING USING KERNEL-BASED EXTENDED DYNAMIC MODE DECOMPOSITION

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In this talk, I will show how kernel-based approximations to the Koopman generator (kgEDMD) can be used to identify implied timescales and meta stable sets in stochastic dynamical systems, and to learn a coarse-grained dynamics on reduced variables, which retain the essential kinetic properties of the full model. The centerpiece of this study is a learning method to identify an effective diffusion in coarse-grained space by leveraging the kgEMD model for the Koopman generator. By combining this method with force matching, a complete model for the effective dynamics can be inferred. We demonstrate that the proposed method successfully and robustly recovers the essential thermodynamic and kinetic properties of the full model for a two-dimensional model system and for benchmark problems in molecular dynamics.