Contribution ID: **45** Type: **Talk**

Approximating Metastable Dynamics with Koopman Operators

Tuesday 18 February 2025 11:30 (30 minutes)

Metastablility is a phenomenon which often inhibits the efficient simulation of dynamical systems, or the generation of samples from high-dimensional probability measures. In particular, metastability is frequently encountered in computer simulations of biological macromolecules using molecular dynamics. It is well-known that metastable transitions and their time scales are encoded in the dominant spectrum of certain transition operators, also called Koopman operators. The study of Koopman operators, and their data-driven approximation by algorithms like the Extended Dynamic Mode Decomposition (EDMD), have gained significant traction in the study of dynamical systems, and have led to widespread application.
In this talk, we will report on recent progress in this field for large-scale systems. First, we will present a study showing that a fairly basic linear dimensionality reduction, combined with a clever design of the basis set, can lead to very accurate Koopman models. The second study we will present is on using equilibrium samples produced by a generative model to feed a model for the Koopman generator. This method allows to extrapolate dynamical properties across different thermodynamic parameters, such as temperature.

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Session Classification: Contibuted Talk