MAX-PLANCK-INSTITUT
FÜR DYNAMIK KOMPLEXER
TECHNISCHER SYSTEME
MAGDEBURG

CSC Seminar

SPEAKER

Hauke Sprink

TITLE

Molecular kinetics with Koopman operators: Application to large-scale systems

ABSTRACT

Transitions between metastable states play a key role in biomolecular function, yet their analysis is difficult due to the high dimensionality of simulation data. Kernel methods are a powerful tool for automated analysis of complex systems, but their need for pairwise kernel evaluations leads to scalability issues in large datasets. To address this, we integrate Random Fourier Features (RFF) into Kernel-based Extended Dynamic Mode Decomposition (EDMD), providing a finite-dimensional approximation of the Koopman operator and a scalable method for the efficient and robust analysis of molecular data.

Tuesday, April 29, 2025 at 2 pm

seminar room Prigogine