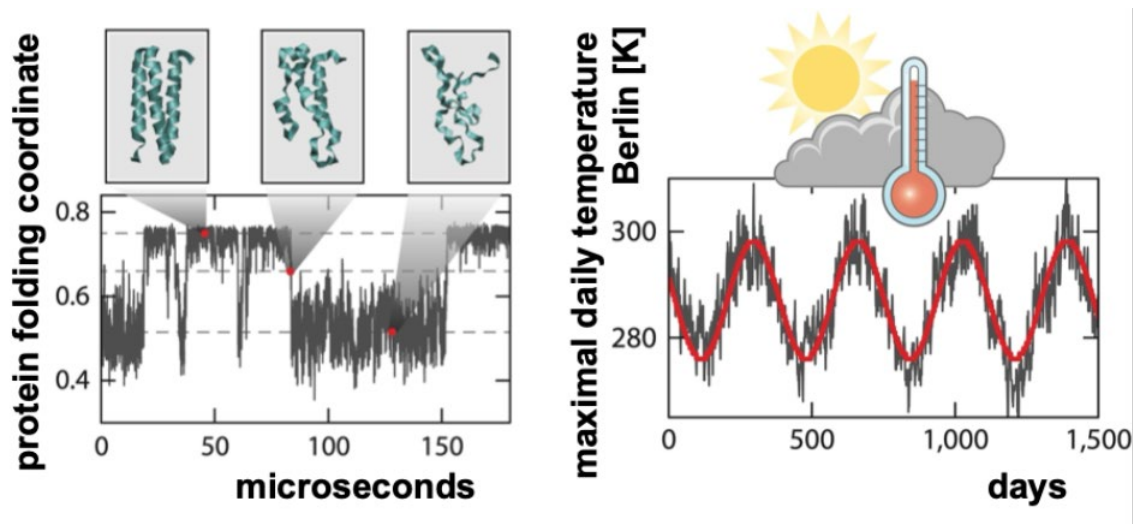


PHYSIKALISCHES KOLLOQUIUM

AM 18. MAI 2026 UM 16 UHR C.T.
IM GROßEN HÖRSAAL



MODELING OF EQUILIBRIUM AND NON-EQUILIBRIUM TIME-SERIES DATA: FROM PROTEIN FOLDING TO WEATHER FORECASTING

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FU BERLIN

The generalized Langevin equation is a non-Markovian equation of motion for general reaction coordinates and derived by exact projection techniques from the Hamiltonian dynamics of a many-body system, it constitutes a systematic coarse-graining approach. A few applications are discussed: From large-scale molecular-dynamics simulations of fast-folding proteins the friction is shown to have memory with a decay time similar to the folding time, leading to anomalous and drastically modified protein kinetics. In fact, folding times are not dictated by free-energy barriers, as predicted by the Arrhenius law, but rather by the non-Markovian friction. Memory effects are also present for non-equilibrium systems. After removing slow and periodic trends from the data by filtering, the GLE can be used to predict complex phenomena such as weather data at a fraction of the numerical cost of machine-learning methods.

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