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Deep Learning in Protein Folding: Trajectory Reconstruction and Ultra-fast Simulators

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Abstract: The integration of data-driven techniques with domain expertise has opened new paradigms and opportunities in understanding and engineering of protein folding. In the first part of this talk, I will describe an approach integrating ideas from dynamical systems theory, manifold learning, and deep learning to reconstruct atomistic protein folding trajectories from one-dimensional time series in experimentally measurable observables. In the second part of this talk, I will describe our development of latent space simulators to perform molecular simulations at six orders of magnitude lower cost than molecular dynamics by stacking specialized deep learning networks to (i) encode a molecular system into a slow latent space, (ii) propagate dynamics in this latent space, and (iii) generatively decode a synthetic molecular trajectory.