Slow dynamical modes from static averages

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We describe the evolution of a complex system not through long trajectories, but via the study of probability distributions evolution. This more collective approach can be made practical using the transfer operator formalism and its associated dynamics generator. Here, we show that the lowest eigenfunctions and eigenvalues of the dynamics generator can be efficiently computed using data easily obtainable from biased simulations. We also show explicitly that the long time dynamics can be reconstructed by using the spectral decomposition of the dynamics operator [1,2]. We will also show the potential of this method for the study of biomolecules. Finally, we will show how the extrapolation behavior of neural networks optimized with a loss based on the dynamics generator allows the discovery of new metastable states.

[1] Timothée Devergne, Vladimir Kostic, Massimiliano Pontil, Michele Parrinello; J. Chem. Phys. 21 March 2025; 162 (12): 124108
[2] Timothée Devergne, Vladimir Kostic, Michele Parrinello, Massimiliano Pontil, Adv. Neural Inform. Process. Syst. 37, 75495–75521 (2024)