FLOW BASED DIMENSION REDUCTION FOR MOLECULAR KINETICS

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Flow-based models, beyond their role as powerful generative tools, offer a principled and flexible approach to dimension reduction in molecular dynamics. In this talk, we present several recent methods that leverage flow-based techniques to extract reaction coordinates and analyze kinetic properties of complex molecular systems. We begin by introducing flow matching approaches grounded in the principles of lumpability and decomposability, which guide the construction of reaction coordinates that preserve essential kinetic features. We then present the reaction coordinate flow (RC flow), a normalizing flow-based framework that yields physically interpretable and invertible low-dimensional representations of molecular systems. Finally, we demonstrate how RC flow can be combined with gentlest ascent dynamics to locate transition states, providing mechanistic insight into rare events and conformational changes. These developments illustrate the potential of flow-based models as effective tools for kinetic model reduction in high-dimensional molecular systems.