

Collective Variables vs Volumes vs Ensembles

CollectiveVariable: snapshot $\rightarrow \mathbb{R}$

What is this dihedral angle?

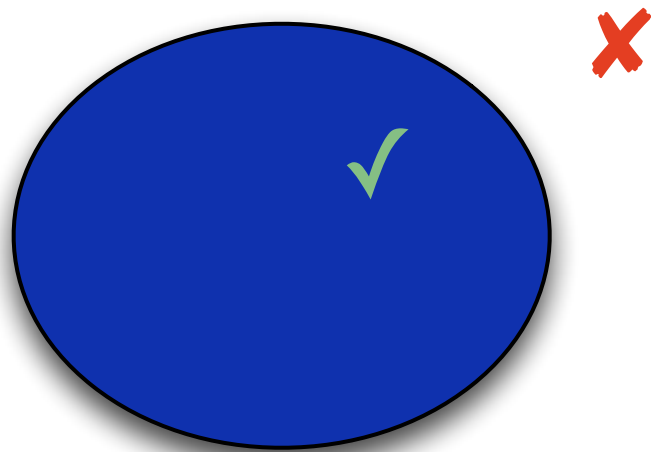
Volume: snapshot $\rightarrow \{T, F\}$

*Is this dihedral angle within the
range that defines the state?*

Ensemble: trajectory $\rightarrow \{T, F\}$

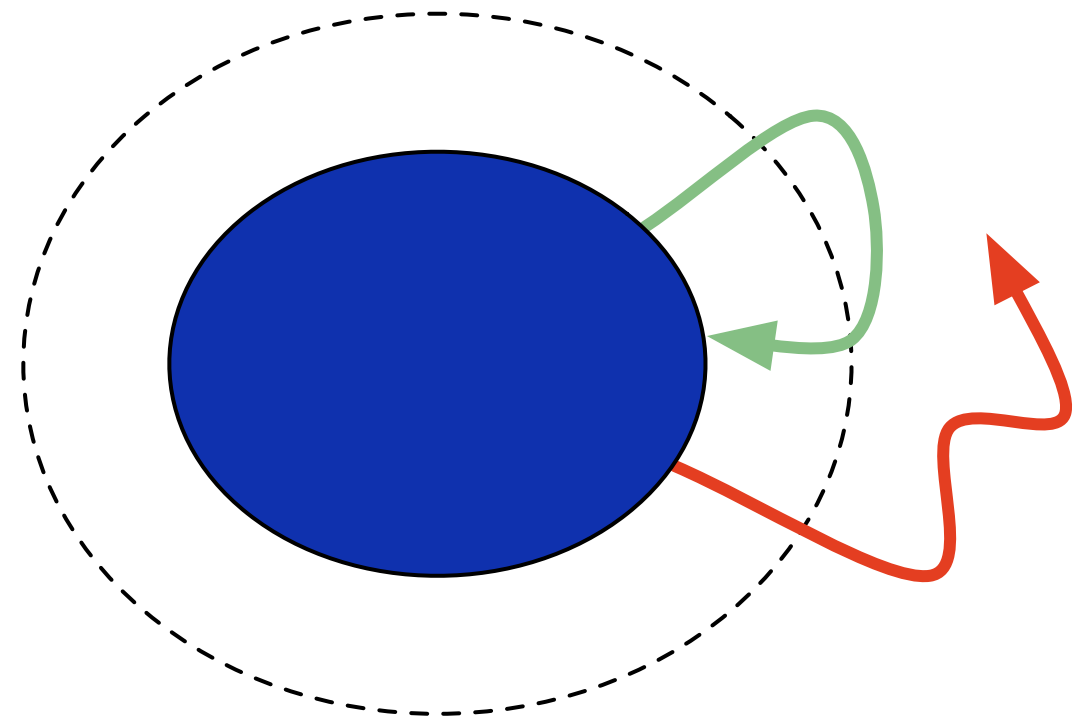
*Does this trajectory change from
one state to another?*

Volumes and Ensembles



Volume: any frame is
either “in” or not

(states, interfaces)



Ensemble: any trajectory is
either “in” or not

(path ensembles)