Path

Simulator

Runnable

Simulation

Collective Variables vs Volumes vs Ensembles

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

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?