

Collective variables in finding transition pathways

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The dynamics of complex systems is often driven by rare but important events. Well-known examples include nucleation events during phase transitions, conformational changes in macromolecules, and chemical reactions. These activated processes occur on a time scale is much larger than the microtime scale in the system. It still remains as a big challenge in simulating molecular dynamics to understand this mechanism. Transition pathways is a core subject in studying rare events. The minimum energy path (MEP) can be viewed as the most probable transition path (MPTP) for smooth landscapes. However, the MEP is difficult to be computed and sometimes it becomes misleading in complex systems. The minimum free energy path (MFEP) provides an alternative way to study it by choosing a new set of collective variables rather than in configuration space. However, no theoretical guidance is available except from limited experiments. We will show an easy and fast algorithm to find the MPTP. Moreover, the standards in selecting collective variables is given.