Homework 9

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What is the key conceptual addition that this group has added to allow one to identify

meaningfully important states in a molecular simulation?

The key addition that the group made was a k-centers clustering algorithm that incorporates both kinetic information and structural similarity. It’s done by dividing the data into microstates, then combining kinetically close microstates into macrostates. To identify the most important states, or representative conformations, the paper suggests several methods. The most basic is calculating the geometric center of a macrostate. Another method proposed is randomly select from a reduced number of conformation from each macrostate. These two methods, however, uniformly select representative conformations, when microstates are not uniformly distributed. The final suggestion is to calculate a list of microstates within each macrostate ordered by density, or probability of a microstate occurring.