# Statistical complexity of classical molecular dynamics systems: a measure of phase space exploration and non-Markovian behaviour of molecular conformation

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Molecular Dynamics simulated trajectories of molecular systems form complex spatio-temporal structures at the picoseconds time scale. Traditional methods of correlation analysis, as well as more advanced approaches based on Takens embedding theorem and surrogate time series analysis [1] used in dynamical systems theory for detecting hidden dynamic correlations in experimental data indicate purely stochastic nature of molecular trajectories. We show that the intrinsic complexity, which is the basis of the formation of molecular structures at much longer time scales, can be quantified using a measure of Statistical Complexity [2–4]. The method estimates the information contained in the molecular trajectory by detecting and quantifying temporal patterns present in the analysed time series. Two types of temporal patterns are found for bulk water molecules. The first is defined by the short-time correlations corresponding to the velocity autocorrelation decay times ($\approx$0.1 ps) and remains unchanged for the time intervals up to the order of tens of nanoseconds. The second is caused by previously unknown long-time correlations (at picosecond time scale) and has complicated dynamics that slowly change with time. Also a direct measure is introduced that describes how the trajectory explores the phase space. The measure is based on the Statistical Complexity and does not depend on the properties of particular molecular system used.

A Molecular Dynamics simulation of the four-residue peptide VPAL (Valine - Proline - Alanine - Leucine) has also been performed. The trajectory is subjected to the Statistical Complexity analysis. This is based on clustering the conformational space into states. The results show non-Markovian memory effects during folding transitions.

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