Analysis and Visual Summarization of Molecular Dynamics

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Molecular Dynamics (MD) simulation is a standard technique used to study the dynamical properties of bio-molecules. The trajectories collected in a MD simulation consists of a very large file containing a serious of 'snap shots' over the simulation time. Analyzing these trajectories may take much longer time than the data generation and the conformational changes may range from small local variation to large displacement of entire domains. Standard parameter like root mean square deviation (RMSD) does not reveal the most interesting properties of the dynamics. Also, managing the large amount of data and presenting them in a comprehensive manner are the major challenges in the analysis part of the MD simulation.

To over come these problems, we use C-alpha torsion angle – pseudo dihedral angle defined by four successive C-alpha atoms [1]- as a parameter. The calculation of differences in C-alpha torsion angles between each steps help to identify the conformational changes without any bias. Hence, we use this approach to identify the local and global conformational changes during MD simulation. To handle the huge amount of data, we use KNIME [2], a user-friendly and comprehensive open-source data integration, processing, analysis and exploration platform.

[1] Maria M. Flocco, Sherry L. Mowbary, Protein Science, **1995**, 4, 2118-2122.
[2] KNIME: The Konstanz Information Miner. (http://www.knime.org)