Multi-way Analysis in Molecular Dynamics Simulations

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The usage of *multi-way* formalism in the analysis of *ab initio* molecular dynamics simulations will be formulated and some preliminaries results presented. Multi-way analysis is well established in some parts of the chemical data analysis (*e.g.* spectroscopy), whereas not so much in quantum chemistry. In particular, the aspect of conformational analysis, which includes collection of structural data from the molecular dynamics trajectories as a sampling method, and tensor decomposition of corresponding multidimensional array of data will be discussed.

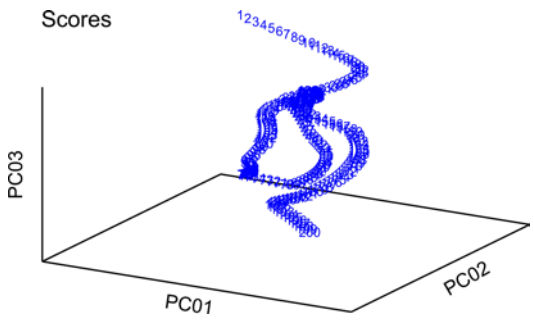

Figure 1: Molecular dynamics trajectory in a reduced space of three principal components.

Results obtained from tensor decomposition allow investigation of molecular dynamics trajectories in significantly reduced space (Fig. 1) and their statistical analysis presents a wealth of information, including full conformational space of the investigated system regardless of its structure.