Singular value decomposition (SVD) of particle movements for motion analysis in cryoEM movies

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Singular value decomposition (SVD) is an efficient method that can be used to find patterns in data. The motions observed in cryoEM movies can be decomposed with SVD, because alignment of multiframes in movies collected in cryoEM SPR provides natural vectorization. The SVD components obtained from such SVD informs how many types of motion are present in a particular experiment.

We developed and implemented efficient SVD decomposition to map the motion features in space and time. SVD can be used as a guided restraint allowing larger motions at the start and dampening them at the later stages. Another use is to filter data for excessive and unusual type of motions, e.g. ice layers collapsing, to allow for automatic data selection for subsequent steps of structure solution. Finally, SVD provides an unbiased, comprehensive, and dataset-specific estimate of the magnitude and character of the largest initial motions driven by ice expansion and bulging. We observed that these highly detrimental initial motions depend on sample features, e.g. particle density, buffer components, and imaging conditions. This approach significantly simplifies motion analysis and make the interpretation more objective.

We will present the results of this analysis for selected cryoEM SPR reconstructions.