# Macromolecular flexibility and its study though the new Zernikes3D bases coupled with MD

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Abstract:

We focus on analyzing macromolecular flexibility from cryo Electron Microscopy images without the constraint that images must come from a discrete set of conformations, which is a paradigm change in the way cryo EM data are currently handled in most cases. We do that by calculating the 3D deformation field and how every image contributes to it, obtaining information of the macromolecule conformational space. The deformation field we obtain is very rich, richer that what dicrete conformations traditional cryoEM software can describe, and it can be explored in a variate of ways, leading to a better understanding of macromolecular motion. Note that this experimental information on conformational landscapes can now be coupled to Molecular Dynamics analysis, trying to capture in this way a notion of time, eventually of “trajectory” and, also, higher resolution atomistic detail. It is currently one of the most porweful frameworks in which to integrate experimental information with computational capabilities. Finally, and not with the goal of flexibility exploration but with the one of helping structural model tracing in difficult cases, we can partially “undo” the so obtained deformation field, increasing the resolution of “motion blurred” areas of the map