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Abstract

Measurement and Minimisation of the Mapping Entropy of a Coarse-Grained Biomolecular System †

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All-atom Molecular Dynamics (MD) is the standard approach to perform in silico simulations of biomolecular systems. Despite its central role in modern computational biophysics, MD cannot span the time scales where the majority of relevant biological processes take place. An alternative is represented by coarse-grained (CG) modelling [1], that is, those lower-resolution representations of the system which aim at effectively reducing the number of degrees of freedom of a biomolecule in order to reach previously inaccessible time scales. Among the several statistical mechanics-based CG'ing techniques, we focused on those that measure the difference in information content between the coarse-grained and the all-atom system. We developed a protocol [2] able to compute the Mapping Entropy, which quantifies the amount of information retained upon the process of CG'ing due only to the choice of the Mapping. Our approach can therefore provide the user with the subset of sites which are maximally informative about the original, fully atomistic system. Tests conducted over a set of well-known proteins showed that regions retained with high probability are often related to the biological function of the molecule.

References

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