Structural regularities, tessellations, and collectivity of folded proteins

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Coarse-grained network models of proteins successfully predict equilibrium properties related to collective modes of motion. In this study, the network construction strategies and their systematic application to proteins are used to explain the role of network models in defining the collective properties of the system. The analysis is based on the radial distribution function, a newly defined angular distribution function and the spectral dimensions of a large set of globular proteins. Our analysis shows that after reaching a certain threshold for cut-off distance, network construction has negligible effect on the collective motions and the fluctuation patterns of the residues.

The results demonstrate that the slow modes are immune to the details of network construction once the essential contacts in the first few coordination shells are included. Thus, the properties that depend on the most collective modes may be studied independent of this choice. Depth dependent analysis, on the other hand, shows that the densely packed core region of the protein has a different local structure built around it compared to its surface. In the core of the protein, the second neighbors have a non-random distribution that is more pronounced than the first neighbors. In the surface residues, the reverse is observed. Specifically, networks constructed by using Voronoi tessellations fail to correctly define the local interactions while they successfully incorporate the long-range pair-wise interactions.