Abstract for GR-TR Conference on Statistical Mechanics and Dynamical Systems

Topic: Complex Networks Preference: Oral

Three-dimensional lattice-based network models portray the properties of folded proteins

Deniz Turgut, Canan Atilgan, Ali Rana Atilgan*

Sabanci University, Faculty of Engineering and Natural Sciences, Istanbul, Turkey
* Electronic Address: atilgan@sabanciuniv.edu

We have previously shown that residue networks that model folded proteins have Ssmall-world T properties (i) with average path lengths that are similar to random nets, but (ii) still retaining local structure [1, 2]. The latter is measured by the clustering coefficient (C), which is a three-point correlation of the neighbors of a given node. While for the distributions of some of the measured properties, such as the path length (L) and connectivity (k) the residue networks resemble the Watts-Strogatz (WS) model (ring lattices randomly rewired with probability $0.01 < \beta < 0.1$), that of C is considerably more peakish. There is also a marked difference between the spectral properties of the normalized Laplacian for the residue networks and the WS model. Moreover, we have found that nearest neighbor degree of a node, (k_{nn}) defined as the average connectivity of nodes with a given connectivity, k, display a striking linear dependence on k, in contrast to the WS model, where there is no correlation. Motivated by these findings, we have investigated the properties of networks obtained from rewired three-dimensional regular lattices. The systems studied are the simple cubic (SC), body-centered-cubic (BCC), face-centered-cubic (FCC) and the hexagonal-close-packed (HCP) lattices. Each of these lattices display small-world properties in the same rewiring probability range of $0.01 < \beta < 0.1$. Their C values are distributed in a more restricted region than WS model, and are similar to that of proteins, BCC being the most peakish. Their k distributions are also different from the WS model, mainly featuring the presence of nodes located at the outermost regions of the three-dimensional lattices. Most strikingly, each has a linear dependence of k_{nn} on k, for a wide range of $\beta = 0$ - 0.5, extending into the region where the small-world properties have been lost. We have further derived a relationship between k_{nn} as a function of C and k under the assumption of constant C for a Poisson distributed network, given by the expression:

$$k_{nn} = Ck + (1 - C)(1 + z) \tag{1}$$

The relationship faithfully approximates the linear dependence observed in the rewired three-dimensional lattice models as well as the residue networks, which all display peakish C distributions. Each of the networks studied has a unique normalized Laplacian spectrum, whose properties with respect to the network structure are discussed.

---

[1] A.R. Atilgan, P. Akan, and C. Baysal, Small-world communication of residues and significance for protein dynamics. Biophysical Journal, 2004. 86(1): p. 85-91.

[2] A.R. Atilgan, D. Turgut, and C. Atilgan, Screened nonbonded interactions in native proteins manipulate optimal paths for robust residue communication. Biophysical Journal, 2007. 92(9): p. 3052-3062.