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Jun-Koo Park* (jun-koo.park@houghton.edu), One Willard Ave., Houghton, NY 14744. *On coarse-grained Normal Mode Analysis and refined Gaussian Network Model for protein structure fluctuations.*

Functions of bio-structures are related to the dynamics, especially various kinds of large-amplitude motions. With some assumptions, those motions can be investigated by Normal Mode Analysis and Gaussian Network Model. However, despite their contributions to many applications, the relationship between NMA and GNM requires a further discussion. In this work, we review the NMA and GNM and evaluate GNM, based on how well it predicts the structural fluctuations, compared to experimental data. Then, we propose ways of coarse-graining for NMA on protein residue-level structural fluctuations by choosing different approaches to represent the amino acids and the forces between them. The residue mean-square-fluctuations and their correlations with the experimental B-factors are calculated for a large set of proteins. The coarse-grained methods perform more efficiently than all-atom normal mode analysis, and also agree better with the B-factors. B-factor correlations are comparable or better than with those estimated with conventional GNM. The extracted force constants are surveyed for different pairs of residues with different extents of separation in sequence. The statistical averages are used to build a finer-grained GNM, which is able to predict fluctuations better than GNM. (Received September 25, 2012)