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Investigation of protein fluctuations via Anisotropic Network Model and Molecular Dynamics[1] OSMAN B. OKAN, DENIZ TURGUT, Rensselaer Polytechnic Institute, ARAVIND RAMMOHAN, Corning Inc., ANGEL E. GARCIA, RAHMI OZISIK, Rensselaer Polytechnic Institute — We use Anisotropic Network Model (ANM) and compare its protein fluctuation predictions against molecular dynamics (MD) simulations and experimental findings for 210 globular proteins. The ANM results are analyzed using bond orientational order (BOO) parameters. We show that BOO parameters could be reformulated as a sum of contact density and geometrical (distribution of contacts in space) components. This reformulation of BOO makes it possible to investigate the role of each individual component separately, and identify cut–off ranges where each component dominates protein fluctuations. Our results indicate that the widely accepted correlation between mean squared displacements (MSDs) and inverse contact density is valid for ANM within the cut-off range of 10–15 Å. We show that the two components of the BOO dominate protein fluctuations at different length scales: contact density at small length scales and geometric distribution of residues at length scales comparable to the protein size. It is also shown that the relationship between MSD and contact density is firmly rooted in BOO, and is rendered possible with a unique distribution of residues that nullifies the average geometric component's contribution to the BOO within the 10−15 Å cut-off.__

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