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Random Matrix Theory Analysis of Molecular Dynamics Simulation

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We apply the random matrix theory [1,2,3] to analyze the time series data of motion of atoms of proteins which is produced by the molecular dynamics simulation [4]. We perform all-atom molecular dynamics simulation with solvent with the maximum duration of 1000ns. We study a data set with the different sampling-time intervals, 0.01fs, 0.1fs, 1fs, 10fs, 100fs, 1ps, and 10ps to observe the characteristic motion at each time scale. The variance-covariance matrices are constructed from the time series data. We calculate the probability density of the variance-covariance matrix, eigenvalue distribution, unfolded eigenvalue distribution of the nearest-neighbor and the next nearest-neighbor level spacings, inverse participation ratio, etc. They are the fundamental quantities which characterize the universality class in the random matrix theory. The results of the nearest-neighbor and the next nearest-neighbor level spacings agree well with the Gaussian orthogonal and Gaussian symplectic ensembles, respectively. On the other hand, the raw eigenvalue distribution has a crossover behavior between the universal and non-universal classes as a function of the sampling-time interval. Following the random matrix theory, we classify the dynamically-correlated sectors of the protein domain by analyzing the eigenvalues outside of the bulk and the inverse participation ratio, and decompose them into subsectors. Our method is an attempt to improve and refine the principal component analysis of protein domain [5].

As an example, we demonstrate our method in the bovine eye lens protein gamma-B (gamma-II)-crystallin, PDBID:4GCR to study the domain decomposition, and ubiquitin carboxy terminal hydrolase L1 bound to ubiquitin vinylmethylester, PDBID:3KW5 to study the protein-ligand and protein-protein dynamical interactions.

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