Title: Using NJIT’s high performance computer center to understand protein aggregation into Amyloid fibrils

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Abstract: In this presentation I will talk about ongoing research in my group to understand at the atomic level protein aggregation into fibril-like structures. Fibrils have wide implications for neurological diseases and for the survival of living organisms. They are main constituents of spider webs that are lightweight yet stronger than steel and silkmoth eggshells that provide protection to developing embryos against environmental hazards. Biological functions of these fibrils are related to the superior mechanical strength of fibrils that persist over a broad range of chemical and thermal conditions desirable for various biotechnological applications. Interest in our group include understanding how the amino acid sequence of proteins affect their propensity to form fibrils and how small molecules when added to aqueous solution affect fibrillization.

A main tool in our lab is all-atom molecular dynamics simulations. We use the GROMACS open source software package that enables parallel computing to perform molecular dynamics simulations. We utilize enhanced sampling techniques that are included in GROMACS (e.g., Umbrella Sampling and Replica Exchange Molecular Dynamics). In this presentation, I will discuss some of the problems we are addressing as well as how we use NJIT’s high performance computer center in our research.