Multiscale Modeling and Simulation of Biological and Polymeric Systems

Balaji Iyer Vaidyanathan Shantha
Swanson School of Engineering, University of Pittsburgh, Pittsburgh, PA-15261

Engineering novel devices with self-regulated intelligent functional response involves seamless integration of materials with multiple components and different properties. Knowledge of structure-function relationships at various length and time scales and harnessing of these relationships to establish specific design criteria is a key requirement to achieve the goal. In view of this requirement, there is an indispensable need for development of sophisticated theoretical and computational models, which could be utilized as valuable tools for designing intelligent multifunctional materials. Recent advances in nanoscale synthesis, functional self-assembly and molecular cell biology has further fueled this demand specifically in macromolecular and biological soft matter systems.

My research interests are in the field of structure-function relationships and multiscale modeling of polymeric and biological systems. This interest stemmed from an intriguing question on dynamics of ring polymers. Notably, the absence of free ends and the complex static structure of ring polymers in presence of topological constraints posed specific challenges different from that of their linear counterparts. I earned my doctorate degree in Chemical Engineering for the study aimed at developing scaling arguments and constitutive relations that connect structure and dynamic response of ring polymeric systems. The experimental verification of some of our theoretical predictions emerged from advances in use of fluorescently tagged DNA strands as model polymers. These advances opened up new exciting avenues for addressing problems in molecular biology from a polymer physics perspective. Specifically, the complex multiscale problem of packaging a meter long DNA within the cell nucleus only a few microns in diameter piqued my interest. I joined Prof. Gaurav Arya's group, Department of NanoEngineering, University of California, San Diego, to devise coarse-grained models for facilitating the study of eukaryotic genome organization within the interphase cell nucleus. Currently, I am seeking ways to combine polymer theory with biologically inspired material design in Prof. Anna Balazs' group, Department of Chemical and Petroleum Engineering, University of Pittsburgh. Computational design of synthetic nanoparticle networks having the desirable features observed in natural dermal armor of animals is the motivation behind this project.

My research goal is to conceive and develop theoretical models and computational tools to establish design criteria for multifunctional and intelligent self-regulated systems at the interface of materials and biology. In this pursuit, I envision the development of multiscale approaches that are inherently multifunctional and can be readily adapted for studying dynamic response. In particular, development of these approaches in synergy with experiments can be valuable to the growth of new technologies that enhance the quality of life. From an academic perspective, the development of multiscale approaches to modeling provides ample opportunities for students to gain a fundamental understanding of interaction between components of a system at different scales, while simultaneously equipping them with the firm knowledge base for developing future technology.

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