Multiscale Modeling of the Nanomechanics of Biomolecular Filaments

by
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Abstract:

Large-size biomolecular systems that assemble, disassemble, and self-repair by controlled inputs play fundamental roles in biology. Microtubules are important in cytoskeletal support and cell motility. Fibrinogen, upon enzymatic conversion to monomeric fibrin, provides the scaffold of blood clots. We focus on deciphering the microscopic origin of the physico-chemical properties of such biological assemblies and the molecular mechanisms of their response to controlled mechanical inputs. Because assemblies have modular architecture and strong inter- and intra-molecular coupling that modulate their properties, any approach has to model them on multiple spatial scales. We developed a multi-scale approach, combining coarse-graining with atomic details, to map out the mechanical properties of large size biological systems on experimental timescales. I will present our results for the micromechanics of microtubule protofilaments, with implications for the mechanism of severing proteins, and our findings regarding the mechanisms of the elongation of fibrinogen protofilaments, in direct correspondence with AFM experiments.

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