# Large-scale Modeling of the Nanomechanics of Biomolecular Shells


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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. Physical properties of capsids of plant and animal viruses are important factors in capsid self-assembly, survival of viruses in the extracellular environment, and their cell infectivity. 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[1,2,3] with atomic details[3,4], implemented on Graphics Processing Units (GPUs) for computational acceleration, to map out the mechanical properties of large size biological systems on experimental timescales. I will present our results for the micromechanics of microtubules[4,5], related to the mechanism of microtubule disassembly, and our findings regarding the link between discrete microscopic transitions and the continuous mechanical response of the Cowpea Chlorotic Mottle Virus capsid at the macroscopic level[6], in direct correspondence with AFM indentation experiments.



**References**

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