Continuum Modeling of Biomolecular Structures

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Modeling biomolecular structures as continuous media has been an attractive and powerful approach to exploring functional mechanisms of, in particular, high molecular weight biomolecules and their assemblies such as molecular transport, binding, and conformational change. Here, we present the finite-element-based modeling approach to investigating the mechanics and conformational dynamics of proteins whose structures are available as either atomic coordinates or electron density maps. We will also briefly discuss the remaining challenges and opportunities for improving the reliability and the efficiency of continuum-based modeling and simulation technologies for biomolecular systems.

Keywords: Biomolecules, Continuum Modeling, Finite Element Method, Mechanics, Conformational Dynamics