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Coarse-grain Approaches to Modeling Biological Macromolecules

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Abstract

Biological problems often involve very large macromolecules, complicated environments, and relatively slow processes. Simulating such systems can be made easier by moving from atomic to so-called coarse-grain representations. However, this requires caution if the basic behavior of the systems studied is not to be perturbed. I will summarize various approaches being developed at the moment and try to point out their advantages and limitations.