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Multiscale modeling on biological systems

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Multiscale modeling on biological systems.

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One of the many challenging and fascinating facets of biological systems is the simultaneous and concerted occurrence of a variety of biochemical and biophysical phenomena spanning many orders of magnitude in time and space. Within the cellular environment, signaling pathways are modulated by hydrogen bonds forming and breaking, enzymatic catalysis, ionic permeation, diffusion, folding, and other phenomena which can be sized from 10^{-10} m to 10^{-5} m and from 10^{-15} s to hours or more. Aimed to address this astonishing complexity, theoretical methods for modeling and simulation of biological systems are constantly being developed. Multiscale methods are gaining popularity because of their capacity to capture relevant details in regions of interest while including the effects of the environment at a coarser and computationally cheaper resolution (G.A. Voth Coarse-Graining of Condensed Phase and Biomolecular Systems CRC Press 2008, Multiscale Modeling of Soft Matter Faraday Discussions 144 (2010)). This requires first, the development of accurate models at different resolutions (i.e., quantum level, classical fully atomistic, coarse grained, mesoscale) and second, the combination of different levels of resolution in a theoretically consistent framework.

In the present issue of BBRC we collected a series of contributions illustrating some of these methods. Applications range from quantum and classic molecular mechanics (QM/MM) (https://doi.org/10.1016/j.bbrc.2017.09.039 , https://doi.org/10.1016/j.bbrc.2017.08.119), theoretical methods to accelerate the conformational sampling in classical simulations (https://doi.org/10.1016/j.bbrc.2017.07.066) to coarse-grained (CG) and multiscale simulations (https://doi.org/10.1016/j.bbrc.2017.08.165). Because of their intrinsic complexity and heterogeneity, special efforts are devoted to the study of membrane systems (https://doi.org/10.1016/j.bbrc.2017.10.132 , https://doi.org/10.1016/j.bbrc.2017.09.040) and the interaction between membranes and proteins (https://doi.org/10.1016/j.bbrc.2017.08.095, https://doi.org/10.1016/j.bbrc.2017.10.164, https://doi.org/10.1016/j.bbrc.2018.01.160, https://doi.org/10.1016/j.bbrc.2018.01.110). Similarly interesting are the CG studies on protein-nucleic acid interactions, which allow for the accurate treatment of large macromolecular assemblies (https://doi.org/10.1016/j.bbrc.2017.09.086) taking into account variations in the charge state (https://doi.org/10.1016/j.bbrc.2017.07.027) and allowing for the accurate backmapping of CG coordinates (https://doi.org/10.1016/j.bbrc.2017.12.057). Finally, an example of stochastic simulation showing a remarkable flexibility to describe a variety of problems is also included (https://doi.org/10.1016/j.bbrc.2017.11.138).

Taken as a whole, the works presented in this special issue provide a broad overview of methods and applications reflecting the capacity of theoretical methods to actually bridge the gap between molecular and computational biology.