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Abstract for an Invited Paper
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Coarse-grained molecular dynamics simulations for giant protein-DNA complexes.

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Biomolecules are highly hierarchic and intrinsically flexible. Thus, computational modeling calls for multi-scale methodologies. We have been developing a coarse-grained biomolecular model where on-average 10-20 atoms are grouped into one coarse-grained (CG) particle (1). Interactions among CG particles are tuned based on atomistic interactions and the fluctuation matching algorithm. CG molecular dynamics methods enable us to simulate much longer time scale motions of much larger molecular systems than fully atomistic models. After broad sampling of structures with CG models, we can easily reconstruct atomistic models, from which one can continue conventional molecular dynamics simulations if desired. Here, we describe our CG modeling methodology for protein-DNA complexes, together with various biological applications, such as the DNA duplication initiation complex, model chromatins, and transcription factor dynamics on chromatin-like environment. (1) Takada, S.; Kanada, R.; Tan, C.; Terakawa, T.; Li, W.; Kenzaki, H. Modeling Structural Dynamics of Biomolecular Complexes by Coarse-Grained Molecular Simulations Accounts of Chemical Research 48: 3026-3035, 2015. (2) Shimizu, M.; Noguchi, Y.;, Sakiyama, Y.; Kawakami, H.; Katayama, T.; Takada, S. Near-atomic structural model for bacterial DNA replication initiation complex and its functional insights. Proc. Nat. Acad. Sci. USA in press.