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Coarse-grained multiscale modeling of proteins and protein complexes

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The traditional modelling based on atomistic molecular dynamics, computational modeling of protein structure, dynamics and interactions remains difficult for many protein systems. It is mostly due to the size of protein conformational spaces and required simulation timescales that are still too large to be studied in atomistic detail. Shrinking the protein representation from all-atom to coarse-grained extends the range of tractable systems. Two levels of coarse-graining and their applicability in the multiscale modeling strategies are discussed. Moderate resolution CABS (C-Alpha, Beta and Side-chain) is already a well-established tool for efficient modeling of protein structure, dynamics and protein-peptide molecular docking. The choice of CABS united atoms for modeling main chains assumes two pseudo-atoms per residue. Side chains are represented by two spherical pseudo-atoms, one centered on Cβ and the other placed in the center of mass of the remaining portion of the side chain, where applicable. The model of interactions used knowledge based statistical potentials and the sampling scheme is based on Monte Carlo dynamics. CABS approach significantly speeds-up the modeling process and generates structures of sufficient resolution for realistic all-atom reconstruction. Unfortunately, CABS and related middle-resolution models are still computationally too expensive for the simulations of large (size and time) systems. For this reason we developed a lower resolution (SURPASS-Single United Residue per Pre-Averaged Secondary Structure fragment) model that still maintains protein-like structural features thanks to knowledge-based sequence specific multibody interaction. SURPASS enables very fast, although of low resolution, simulations of large proteins and protein systems. Multiscale modeling strategies based on combination of these coarse-grained models are briefly discussed.

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