Methodological advances in computer simulation of biomolecular systems

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Computer simulation of the dynamics of biomolecular systems by the molecular dynamics technique yields the possibility of describing structure-energy-function relationships of molecular processes in terms of interactions at the atomic level. Yet, the time and spatial scale of simulations is limited due to finite computing power. Recent advances in simulation methodology e.g. to rapidly compute many free energies from a single simulation, to use experimental data in a non-biasing manner in simulation, or to extend the time scale of simulation by coarse-graining will be discussed.

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