Development of hybrid method of representing proteins.

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In the last 25 years the molecular dynamics method has become an important tool in science, especially in biotechnology. Molecular dynamics is used, for example, for investigation of such phenomena as the conformational changes of proteins, interactions between molecules and for refinement of protein X-ray structures. Simulations of bigger systems, such as viral capsids, are possible, but not viable due to the huge amount of required calculations. One of the ways of decreasing the number of calculations, therefore speeding up the simulations, would be to decrease the number of atoms in the simulation.

The Coarse-grained modeling is a set of methods which aim to simulate the behavior of large, complex systems by simplifying biomolecule structure. This is achieved by representing groups of atoms in a biomolecule with a pseudo-atom – a construct whose charge and mass is equivalent to mass and charge of atoms it represents. The downside of *coarse graining* is the decrease of resolution as well as the loss of the insight into most interactions between biomolecules.

The hybrid method of representing proteins aims to allow for the investigation of complex systems while taking into account the interactions between protein molecules. This will be accomplished by representing most of the protein amino acid residues using the *coarse grain model*, while the amino acid residues responsible for the interaction between proteins will be represented in atomistic resolution.