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Implementing a modeling software for animated protein-complex interactions using a physics simulation library

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Abstract

To better understand the behaviors and structural dynamics of proteins within a cell, novel software tools are being developed that can create molecular animations based on the findings of structural biology. This study proposes our method developed based on our prototypes to detect collisions and examine the soft-body dynamics of molecular models. The code was implemented with a software development toolkit for rigid-body dynamics simulation and a three-dimensional graphics library. The essential functions of the target software system included the basic molecular modeling environment, collision detection in the molecular models, and physical simulations of the movement of the model. Taking advantage of recent software technologies such as physics simulation modules and interpreted scripting language, the functions required for accurate and meaningful molecular animation were implemented efficiently.