C-1-20

Development of molecular modeling software for protein complex animations

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Keywords: Protein modeling, Protein Complex animation

For understanding functions of protein molecules the atomic coordinate data allows us to model the interacting protein complex. In addition to the experimental evidence for the molecular interactions, there are molecular dynamics studies for analyzing works of a protein complex. Since these techniques are the analyses by theoretical calculation based on a hypothesis of working mechanism, it is difficult to discover how the complex is actually working. Thus, the demand of making animated models of the protein complex has increased. Such tasks involving two or more existing software tools alternatively are usually not trivial. For these computational problems, we started a software development of the script editor to facilitate making animations of molecular models visualizing molecular simulations and the protein interactions. The implementation of this software was greatly supported by a graphical software development tool, Luxinia. It is also known as a game engine incorporating Open Dynamics Engine (ODE) for the physical simulation and the graphics library OpenGL by means of Lua, a quick scripting language. Our software development is ongoing for the molecular model arrangement functions required for creating animations, a time-line editor, and a simulation facility, while the function for the photorealistic rendering is omitted at first. Our development aims to clarify necessary functions required for making molecule animations for the researchers in molecular biology. The efficiency in improving and extending the software is reinforced by the scripting language that allows adding custom functions for individual researchers to animate protein molecules to fit their experimental results easily.