Using 3D Animation Software for the analysis of protein motion

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Motivation

The description of biological processes at the cellular and molecular level has reached a level of unprecedented details in terms participating objects (proteins, nucleic acids and cellular organelles) and the biochemical principles that govern them. The last few years have also seen impressive advances in the development of computer graphics and 3D animation. We think that the time is now mature to propose a vision of life at the nanoscale in 3D animation, importing and processing molecular data, in particular protein structural data, in 3D animation software, such as Autodesk® Maya or Blender. Using these tools, it is possible to visually represent molecular events in a meaningful way, modelling proteins according to the experimentally determined atomic co-ordinates, and moving them respecting chemical and physical principles. We are building tools that make it possible for scientists to observe directly the kinetics and conformational changes of the proteins object of their study.

Methods

We show here some results obtained using the software Blender, an Open Source package for the modelling and animation in 3D. A script to import and export pdb data with multiple models (from NMR analysis) in the software has been implemented. Animation (i.e. transition between imported conformations) is achieved by using internal Blender engine, equipped with a set of rules that mimic natural behaviour. Validation of new structures obtained is made using Swiss_Pdb viewer which implements the GROMOS force fields, and by RMSD calculi between published and newly obtained structures.

Results

The 1cfc pdb file, which contains 25 NMR conformations of Calmodulin, without Calcium nor bound peptide, has been imported in Blender. We will present the animation obtained with our program in Blender, and demonstrate that the calculated molecular movements are compatible with experimental data. We also propose some visual elaborations of surface properties such as electrostatic potential and lipophylicity, realized using Blender render engine.

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