Use of BioBlender for all atom morphing of protein structures

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Motivations

The vast majority of proteins and other biological macromolecules act in life processes through some form of motion. While this concept has been recognized and is ever more considered in the structural biology field, it is still difficult to handle by the majority of experimental scientists. We reasoned that a simple system that enables biologists to elaborate protein motion would help experimental scientists to better understand the complex spacial behavior of proteins.

Methods

Using Blender, a complete package for Computer Graphics, Gaming and Visual effects, we have developed BioBlender, which uses the game engine for interpolation between different conformations of a proteins. The conformations can be derived from studies of NMR, or can be calculated according to Normal Mode Analysis. The system can be downloaded as a stand alone and we are also preparing a server for the elaboration of complex that contain large N of atoms (> 10.000). Elaboration of motion is performed using the Game Engine embedded in Blender, equipped with a set of rules that mimic the main features of chemical motion, i.e. that atoms can move by rotation of the previous bond (implemented by allowing rotation on torsion angles only), and that atoms cannot occupy the same space at the same time (collision detector).

Results

The motion was recorded and exported in .pdb format as a series of conformations trajecting the molecule between the two given models. Evaluation using the GROMOS force filed in Swiss PDB viewer revealed a very good agreement with data derived experimentally, and /or calculated using classical Molecular Dynamics simulations.

Availability

http://www.bioblender.net/