Fast elaboration of motion and intuitive visualization of surface properties of moving proteins

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Motivation

The availability of protein structures enables the study of their surfaces and surface properties such as electrostatic potential (EP) and hydrophobicity (MLP), based on atomic contribution. Recently, it has become possible to observe also protein motion, elaborated with studies of Molecular dynamics, via Normal Mode Analysis, by elastic network, or using a morphing system based on interpolation between known structures. The observation of protein in motion, however, is still unsatisfactory: present visualization tools can show dynamically only a limited number of atoms, typically main chain or a subset of atoms in the reactive site. We have engaged in the elaboration of motion and in the study of a visualization system that permits the observation of animated proteins with the simultaneous representation of molecular surface (determined by all atoms), with its Lipophilic and Electrostatic potentials.

Methods

Recent advances in 3D animation and rendering software have not yet been exploited for the representation of proteins and other biological molecules in an intuitive, animated form. Taking advantage of Blender, an open-source, 3D animation and rendering software, we elaborate proteins' motions between different conformations and visualize EP and MLP for every conformational transition of the protein. EP and MLP are calculated using chemico-physical programs and custom programs and scripts. A new code is introduced for MLP visualization: a range of optical features that goes from dark-dull-rough surfaces for the most hydrophilic areas to bright-shiny-smooth surfaces for the most lipophilic ones. This kind of representation permits a smooth spatial distribution of the values of MLP on the surface of the protein. EP is represented as animated line particles that flow along field lines from positive to negative.

Results

Our system permits the fast morphing of proteins, elaborating transition between conformations in a fast and reliable way, using Blender Game Engine. Once obtained the sequence, we propose protein visualization as an animated video in

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which the molecule is shown as surface, rather than structure. EP and MLP are shown simultaneously for each intermediate conformation of moving proteins avoiding the use of color, which cannot be interpreted without a legend. Using real world tactile/sight feelings, the nanoscale world of proteins becomes more understandable, familiar to our everyday life, making it easier to introduce “un-seen” phenomena (concepts) such as hydropathy or charges, while leaving the utilization of color space for the description of other biochemical information. Example of a movie showing Calmodulin fluctuating between NMR conformations in its Apo form (unbound) and transiting to a Ca-bound form (4 Ca ions binding to the EF hands) can be seen from our website or in Proteopedia (www.protpeopedia.org)

Availability
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Image