SORS: BioBlender: 3D Computer Graphics for Structural Biology

Speaker: Monica Zoppè (Inst. of Clinical Physiology, National Research Council, Pisa)

Abstract: Recent advances in highly performant investigation methods contribute to obtain information about cells, from molecules to tissues, acros 4 orders of magnitude: from cell shape and composition to atomic structure of macromolecules. Our aim is to integrate available information about biomolecules activities and present them in an intuitive, animated form (www.scivis.it). The cellular environment and its components are recreated in Blender, a free, open-source, 3D modelling, animation and rendering package.

We focused on atomic scale visualization and developed BioBlender (www.bioblender.eu), a package dedicated to biological work, that comprise two major features: elaboration of proteins' motions using the game engine and the simultaneous visualization of physico-chemical features on molecular surface.

Blender's Game Engine is used to calculate protein motions by interpolating between different conformations according to specific rules. Transition between NMR collections or different X-rays structures of the same protein are obtained, as physically plausible sequence of intermediate conformations that are the basis for the subsequent visual elaboration.

A new visual, photo-realistic code, is introduced for MLP visualization: a range of optical features, from dull-rough-dark surfaces for hydrophilic areas to shiny-smooth-clear for lipophilic.

EP is represented as animated line particles that flow along field lines, from positive to negative, proportional to the total charge of the protein.

BioBlender is a new and fast system to calculate conformational changes of proteins between known conformations. It also includes a novel code for their intuitive representation, which contributes to gain insight into the function of molecules by drawing viewer's attention to the most active regions of the protein. A more direct visualization can result in an increased understanding of biological activities.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación