

## **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, across 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](http://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](http://www.bioblender.eu)), a package dedicated to biological work, that comprises 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 a 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.

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