Representation of surface properties of bio-molecules using BioBlender

Introduction

In living cells proteins are continuously in movement. Two protein properties which have a vital rule in motion and interaction with other proteins or other mediums are the electrostatic and lipophilic-potential. There are many physico-chemical programs for the calculation of these features which supports the visualization as range of colors. But as there exist various types of color-codes, understanding of them require proficient eye and, at the same time it is usually not possible to color-code difference feature simultaneously.

With BioBlender a new visual-code is introduced for Molecular Lipophilic Potential (*MLP*) in which a range of optical properties are encoded from smooth-shiny surface for hydrophobic regions and rough-dull one for hydrophilic regions. Electorstatic Potential (*EP*) is shown as small particles that flow alongside the field lines which depends to the charge of the protein (Figure 1)

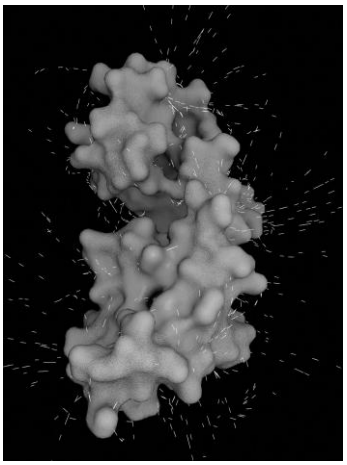

Figure 1

BioBlender

BioBlender is a software package built on top of Blender.

With BioBlender we can handle proteins in the 3D space, display their surface in a photorealistic way, and elaborate protein movements on the basis of known conformations. It is also possible load PDB files and visualize them in 3D, calculate and show its surface features(MLP, EP). Output files are exported in PDB format, and images as movie that can be used to show physical as well as chemical features as molecule in motion(Figure 2).

In BioBlender custom Python scripts have been employed for building the interface, importing the meshes and the curves, converting MLP values into vertex colors and running various scientific programs such as:

- Blender
- PyMOL
- PDB2PQR
- APBS (Adaptive Poisson-Boltzmann Solver)
- Python 2.6

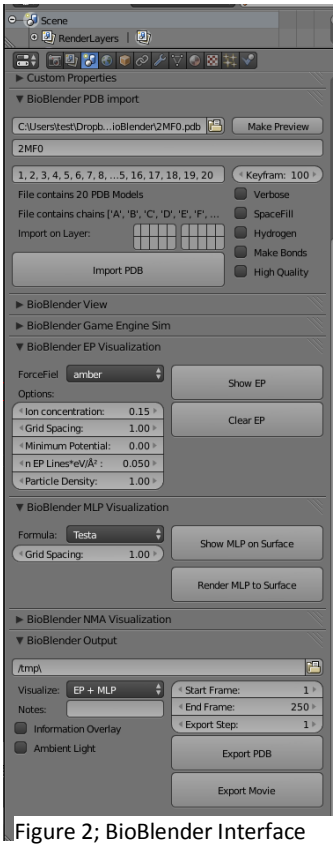

Figure 2; BioBlender Interface

MLP Function

For each .pdb file, PyMOL and pyMLP.py calculate the surface and the MLP values, respectively; then, MLP (stored in a .dx file) is mapped onto the surface and both are saved as an .obj file; MLP values are converted into vertex colors, and texture images are saved. These are finally mapped onto the material of the mesh, and rendered as bump and specular effects (Figure 3).

EP Function

For the same .pdb file used for MLP calculation, PDB2PQR adds a specific atomic charge to each atom. Then APBS calculates the EP values and stores them in a .dx file. Scivis uses the information about

the mesh (before calculated for MLP) and the .dx file to calculate the field lines. These file are imported in Blender as curves along which the particles travel. emitted from their positive end.

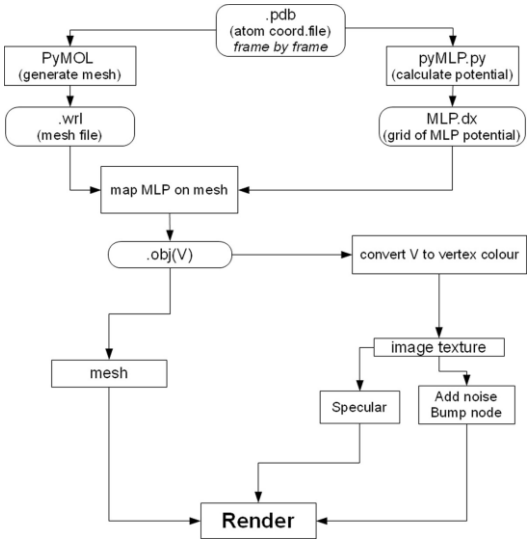

Figure 3; Molecular Lipophilic Potential (MLP)

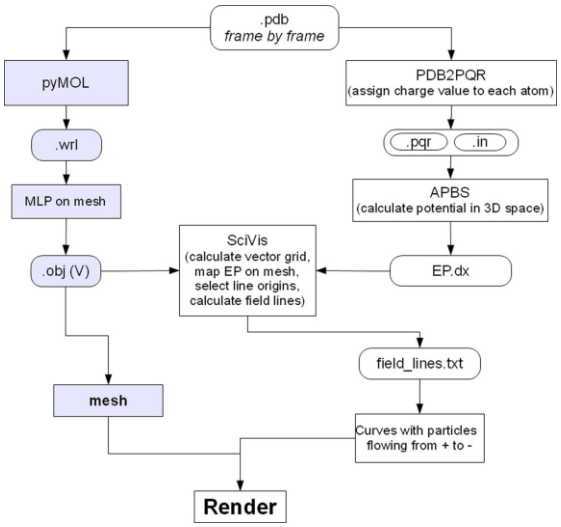

Figure 4; Electrostatic Potential(EP)

Availability

The software is freely available from http://www.bioblender.eu for Windows, and Linux

References

Andrei R.M. et al. Intuitive representation of surface properties of biomolecules using BioBlender. BMC Bioinformatics 2012, 13(Suppl 4):S16. Published: 28 March 2012
Andrei RM, Pan CM, Zoppè M: BioBlender: Blender for Biologists. *BlenderArt Magazine* 2010, 31:27-32

Callieri M. et al. Visualization Methods for Molecular Studies on the Web Platform (The Web3D 2010 Conference 15th International Conference on 3D Web Technology, 22 – 24 July 2010, Los Angeles, California)

Zoppè M. et.al. Blender for biology: The making of Protein Expressions – Study N.2 (Proceedings of the Blender Conference 2009, 22 – 26 October 2009, Amsterdam, the Netherlands)
BioBlender http://www.bioblender.eu