

Beyond computation, the representation of electrostatics in biological settings

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Abstract

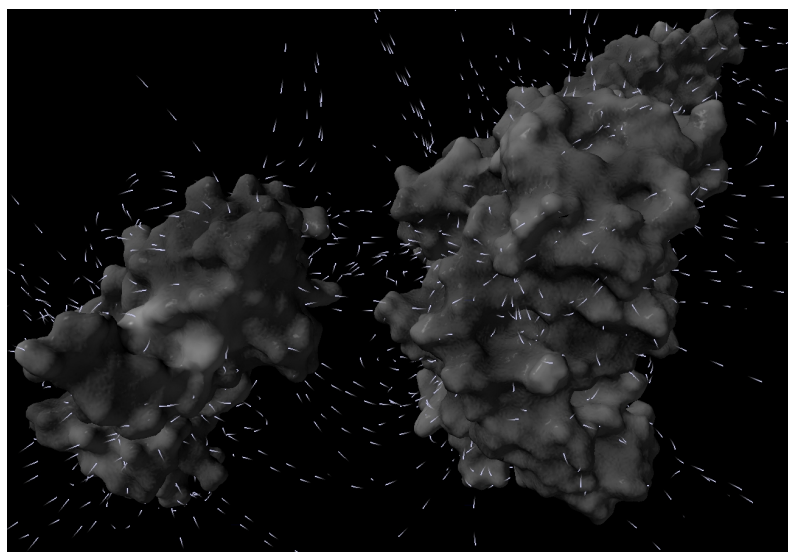
The Scientific Visualization Unit of IFC, CNR, has developed BioBlender, a tool that offers 2 groups of capabilities: the 'quick and dirty', approximate calculation of protein motion, operated by the Blender Game Engine on the basis of two or more given protein conformations, and the representation of bio-molecules (in single conformation or in motion) using a specifically developed visual code. This second feature transform atomic information (PDB) to a molecular surface capable of delivering also information on its lipophilic and electrostatic potentials.

In particular, for the visualization of the Electrostatic Potential (EP), BioBlender uses PDB2PQR and APBS to calculate the values in the volume of and around the molecule, organized in a grid with user-set spacing. These values are sent to an algorithm that interpolates with the protein surface, transforms the grid of values in a grid of gradients, selects the most active areas on the surface of the molecule using a Monte Carlo sampling, and draws the field lines. These are encoded as series of points in a txt file and finally sent to BioBlender for rendering.

The two most widely used visualization techniques used to show the values and distribution of EP in and around the space of a protein are the drawing of isosurfaces, typically color-coded, and the drawing of field lines. We chose to elaborate the lines, since it is not easy, for human beings, to evaluate the steepness of a surface in a 2D representation, even using the most sophisticated techniques that use semi-transparent surfaces or volumetric representations.

The rendering of EP that we propose is composed of small, thin lines that run along the field lines, from positive to negative. In this way, while the direction of the field is immediately conveyed by the motion of the particles, the intensity of the field is perceived thanks to the number of lines, all in the same part of the volume. Since all lines start or end at the molecular surface, it also become immediately evident where precisely on the protein are located the charged residues that mostly influence the field.

This representation is of particular value when used in the study of interaction between two molecules. An example is given in the figure (where the small lines are substituted by comets in order to provide directional information even in a single image), representing the approaching of Ca-Calmodulin to one of its target, Myosin light chain Kinase (MLCK). The image is a screenshot of the interactive application, based on BioBlender visual code and WebGL, SpiderGL.



Other examples will be shown at the meeting.

http://www.scivis.ifc.cnr.it/images/stories/3d_interactive/VIS_CaCaM_MLCK/VIS_CaCaM_MLCK.html