Representation of surface properties of biomolecules using BioBlender

Multidimensional Cell Visualization

Mohammad Rafi Noori

12.06.14

Contents

- Overview
- Objective of BioBlender
- Packaging and installation
- General workflow
- User interface
- Out look

Overview

- In living cells, proteins are in continuous motion and interaction with the surrounding medium
- These interactions are mediate by electrostatic and lipophilic potentials.
- Calculated by physico-chemical programs and visualized as range of colors

Overview

- Color coding vary according to the tool
- With color code, encoding of characterestic and simultaneous visualization is almost impossible
- Require knowledge to decrypt color code

Objective of BioBlender

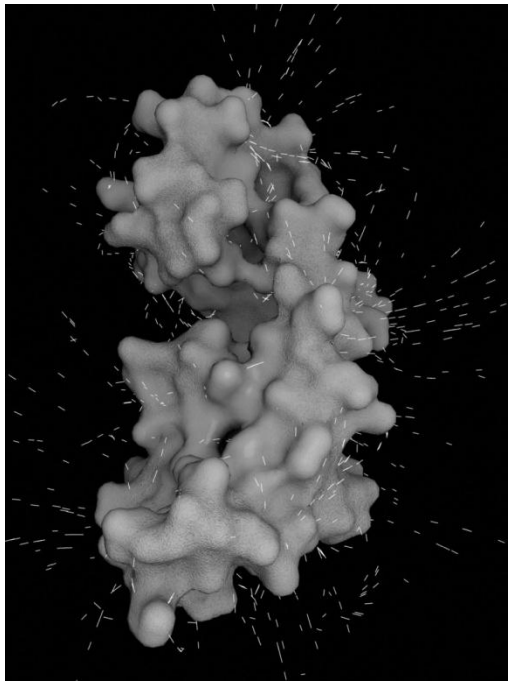
- Many tools for the visualization of 3D structures
  - VMD
  - SPDBViewer
  - Chimera
  - PyMOL and more
- Most of them can also calculate surface features such as **electrostatic potential EP**.
- These features are shown as field lines or as ranges of colors.

Objective of BioBlender

- With 3D animation and rendering open-source software a novel and intuitive code
- Bio Blender to show simultaneous visualization of chemical and physica properties.
- EP and MLP are calculated using some software and scripts, accessed through BioBlender interface.
- Example

Objective of BioBlender

- MLP is a range of optical features going from smooth-shiny for hydrophobic regions to rough-dull for hydrophilic.
- EP is shown as animated line particles that flow along field lines.
- Aim is to visualize molecules in a directly informative way



Programs and scripts

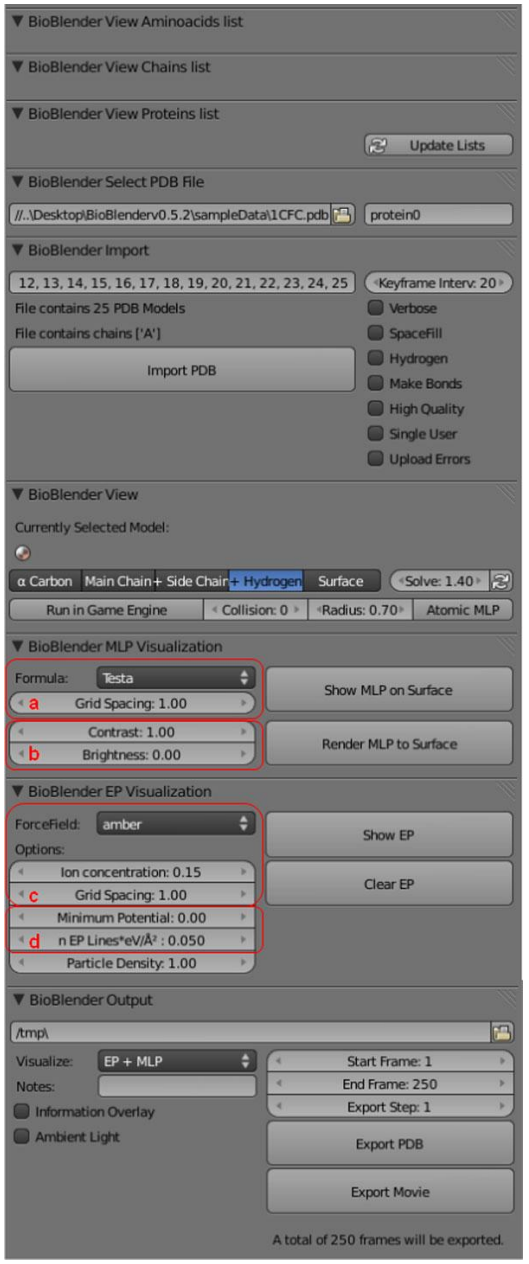
- Programs in the construction of BioBlender
  - **Blender:** is a free, open source, cross platform suite of tools for 3D creation
  - **PyMOL:** is a molecular graphics tool, used for visualization of .pdb files. It calculates the electrostatic potential through APBS plug-in.
  - **PDB2PQR:** providing a utility for
    - Converting protein files from PDB format to PQR format.
    - Assigns partial atomic charge to every atom according to different force fields.
  - **APBS:** is a software for evaluating the electrostatic properties of nanoscale biomolecular systems

Programs and scripts

- **civis.exe:** is a software to calculate the field lines and to export them in a ASCII, it imports the 3D surface (.obj) and the EP grid (.dx) calculated by APBS.
- **Python 2.6:** is an interpreted, interactive, OO, extensible programming language.
- **pyMLP.py:** is a Python script that contains a library of atomic lipophilic potential for all atoms present in proteins

BioBlender Interface

- BioBlender is used to
  - access several mentioned scientific programs.
  - biological visualization
  - handle proteins in the 3D space
  - displaying protien surface in a photorealistic way

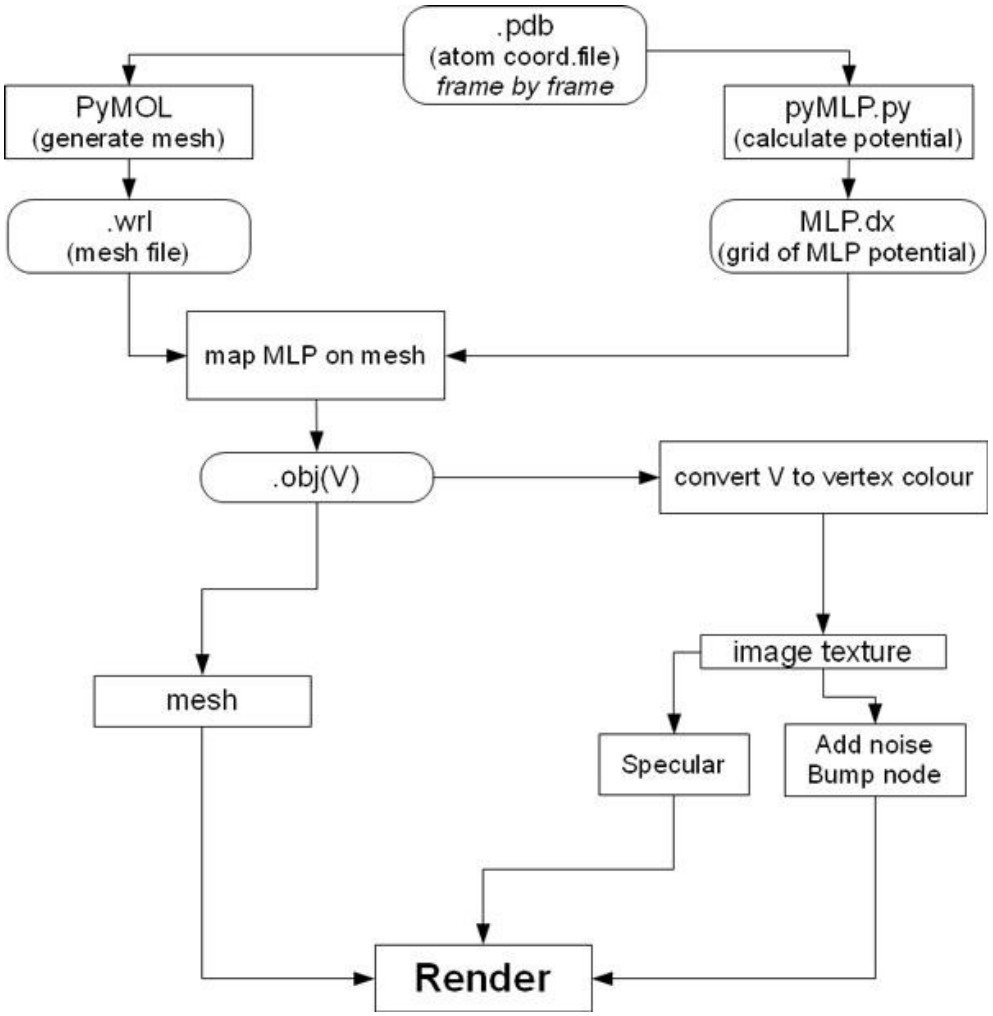


MLP calculus and representation

- PyMOL and pyMLP.py calculate the surface and the MLP values of PDF.
- MLP (in a .dx file) is mapped on the surface and both are saved as an .obj file.
- MLP values are converted into vertex colors, and texture images.
- These are finally mapped on the material of the mesh, and rendered as bump and mirror-like effects.

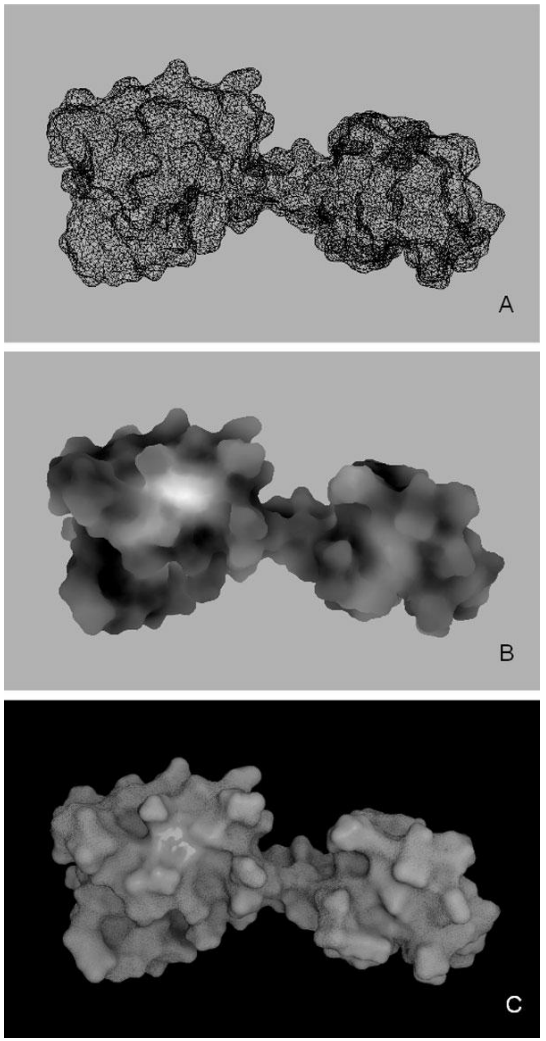
Diagram in next slide…

MLP calculus and representation



MLP mapping on surface of Calmodulin

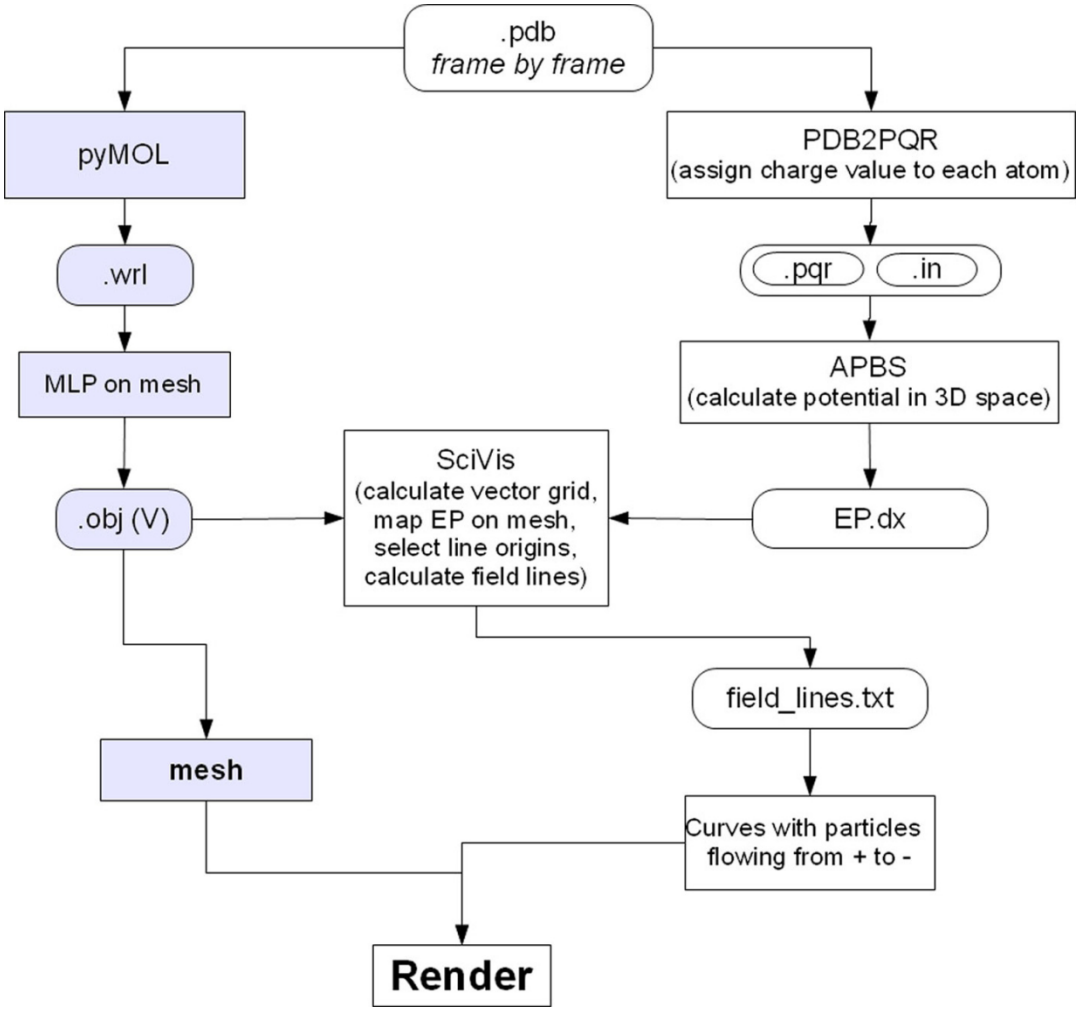
- Steps in the creation of an image of Calmodulin:
  - A) Panel of the 3D scene of Blender with a wireframe view.
  - B) MLP representation as levels of grey.
  - C) Final image showing the variation of MLP distribution over the molecular surface.



EP calculus and representation

- Take the same .PDB file used for MLP calculation
- PDB2PQR adds atomic charge to each atom
- APBS calculates the EP values and stores them in a .dx file
- Scivis uses the information about the mesh (previously calculated for MLP) and the .dx file to calculate the field lines
- Finally imported in Blender as curves along which travel particles, emitted from their positive end

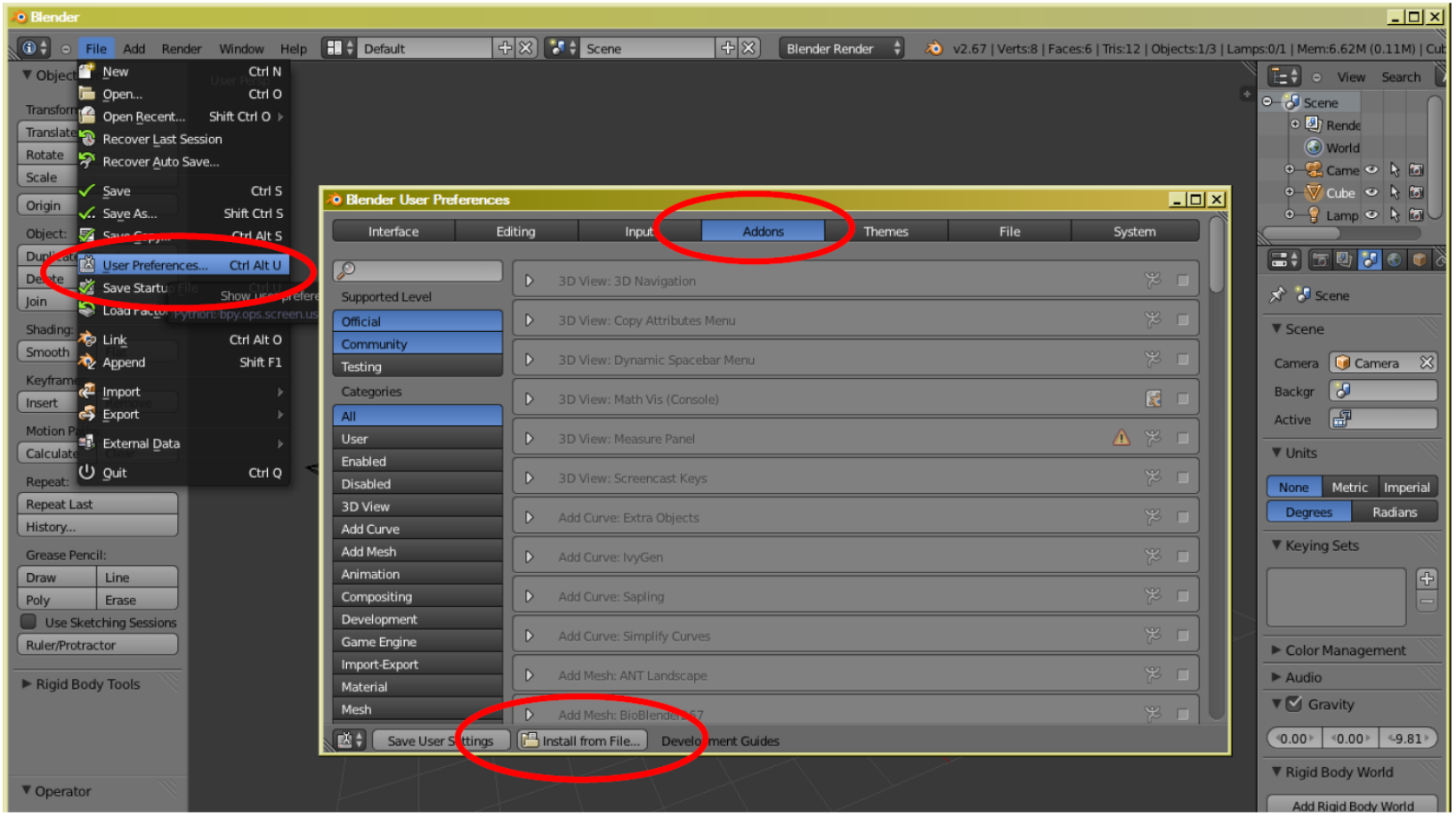
EP calculus and representation



Packaging and Installation of 1.0V

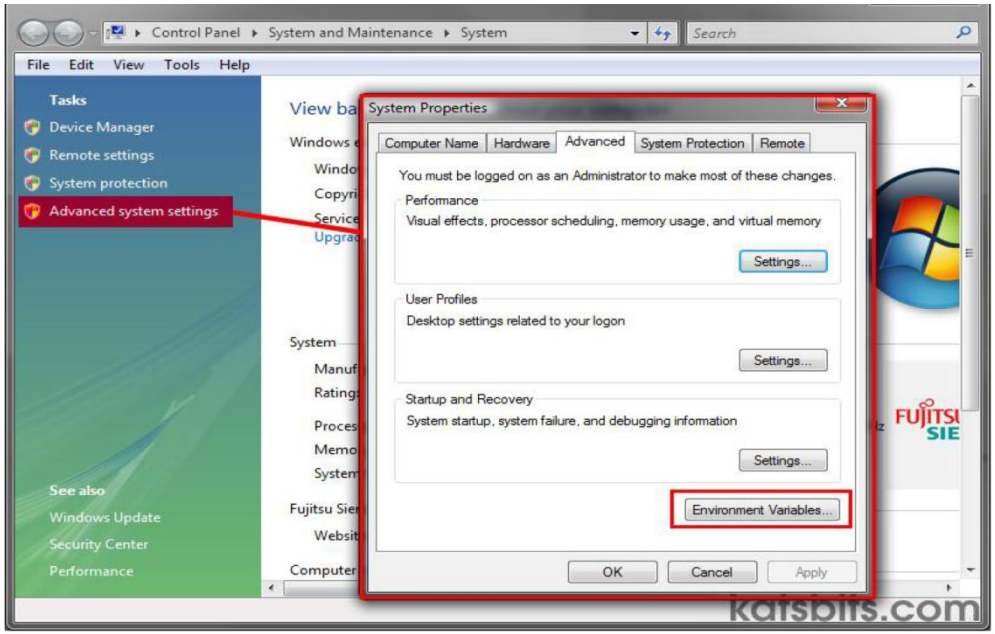
- This new version is released as an add-on to the Blender
- BioBlender needs a few other software packages installed like
  - Blender 2.67 or newer
  - ProDy
  - PyMOL
  - Python 2.6 or 2.7
- Download BioBlender 1.0, zipped (do not extract)
- Open Blender and go to the User Preference panel select tab Addons, click Install from file.

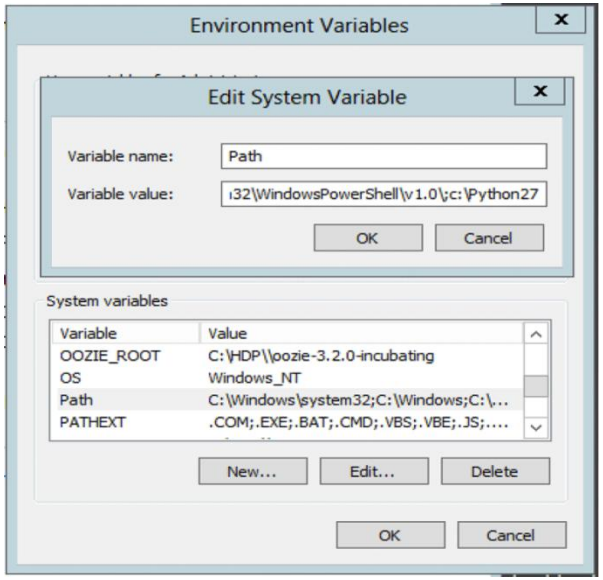
Packaging and Installation of 1.0V



Packaging and Installation of 1.0V

- For MS Windows set the Python PATH in Environment Variables (e.g: *;C:\Python26*)





General Workflow

- The BioBlender user interface is contained in the vertical Scene Property Panel.
- Import, export, view, and manipulate the molecular data.
- Each interface element (buttons, sliders, toggles) has help text associated with it (
- Errors and progresses are displayMouse-over)ed in the console window.
- Critical errors will appear in the main BioBlender Interface as a popup.

General Workflow

1. Select a PDB file and set the desired import options
2. PDB Import
   - Select file
   - Make preview
   - Import PDB
3. MLP Visualization
   - Show MLP on Surface calculates the lipophillicity of the molecule on the surface.
4. EP Visualization
   - Show EP
   - Options
   - Force Field

General Workflow

- The timeline at the bottom of the BioBlender shows the progress of the animation.
- Animation will start playing automatically once the import process is complete, but not in new version.
- length of animation = the number of conformations x the key-frame interval
- Running the EP visualization will also animate in the 3d viewport.(the particals)

Demo

Outlook

- Version 1.0 has some problems in two major features
  - It cannot import proteins of medium to large size
  - Cannot calculate MLP.
- For this reason this features have been withdrawn, while they look for solutions to the problems.
- Game Engine is not working properly in V1.0

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- SciVis Unit http://www.scivis.it/videos/
- PDB http://www.pdb.org/pdb/home/home.do

Thank you