A Short Introduction to PMV-Vision and Applications to EM

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This tutorial provides a brief introduction to the MGLTools software package. More specifically, we will present PMV: a fully fledged molecular visualization tool, and Vision: a visual programming environment (formerly known as ViPEr). We will briefly tour the interface, basic operations and demonstrate the manual fitting a crystallographic structure into a cryoEM map.

References:

- *"ViPEr, a visual Programming Environment for Python.*" In Proceedings of the 10th International Python conference. 103-115. February 4-7, 2002. ISBN 1-930792-05-0

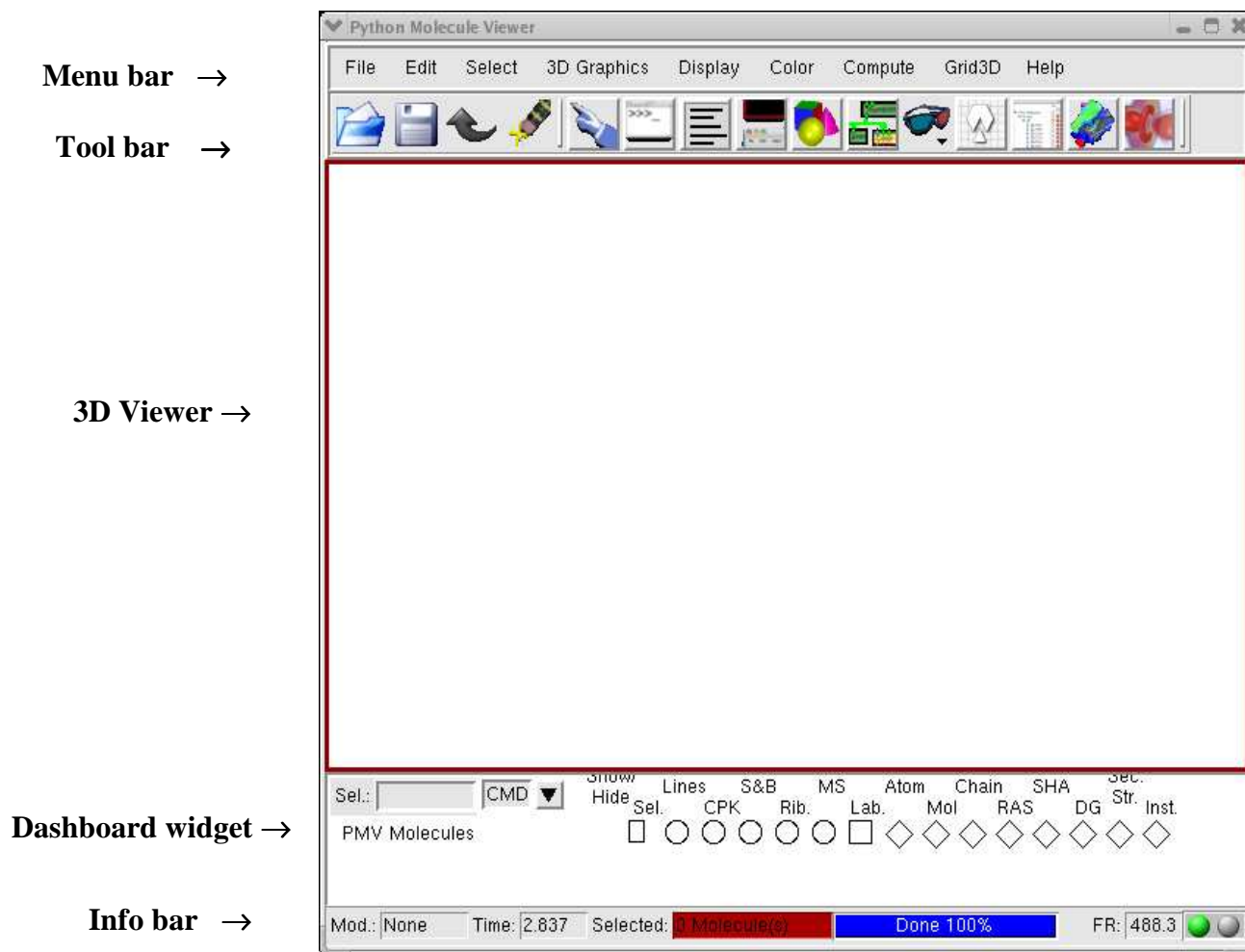- "A component-based software environment for visualizing large macromolecular assemblies." Structure. 2005 Mar;13(3):447-62

reprints can be found at "docs" subdirectory.

Installation

Visit http://mgltools.scripps.edu for latest release, news and documents. Installers are available for Linux, MacOS and MS Windows. Bug reporting and user mailing list are also available.

PMV and the 3D Grid Rendering Control Panel.

Menu bar →

Tool bar →

3D Viewer →

Dashboard widget →

Info bar →

Read Session		Float Camera
Save Session		DejaVu GUI
Undo		Vision
Clear Selection		Toggle Mono/Stereo
Picking Commands		AutoDockTools
Python Shell		Cartoon Rendering
Message Box		Volume Rendering

Please find the latest PMV tutorial under "docs" directory.

Exercise 1: Visualize a molecule

1) right click the "PMV Molecules" label in Dashboard widget

2) choose "1crn.pdb" and PMV loads the molecule.

Try to interact with the molecule. See the following table for the summary of mouse operations.

Button Mod	Left	Middle	Right
None	*Pick*	*Rotate*	*Translate left/right (X) and up/down (Y)*
Shift		*Scale or Zoom*	*Translate in/out (Z)*

On Apple Computers:.

`option`: Rotate

`command`: Translate left/right

`shift`+`option`: Scale or Zoom

`shift`+`command`: Translate in/out

3) try to turn on/off the display modes by clicking the circles on the dashboard, such as lines, CPK, Stick-and-ball (S&B), secondary structure (Rib) and molecular surface (MS).

4) try to color the molecule by different schemes such as by Atoms, by Molecule (when multiple molecules are loaded), by chain, by residues (Rasmol or Shapely), by David Goodsell's scheme, by secondary structure types and by instances.

5) right click the "1crn" caption on the dashboard and click "delete" to remove this molecule from PMV

Vision

Start vision by clicking the [icon] icon on the PMV toolbar.
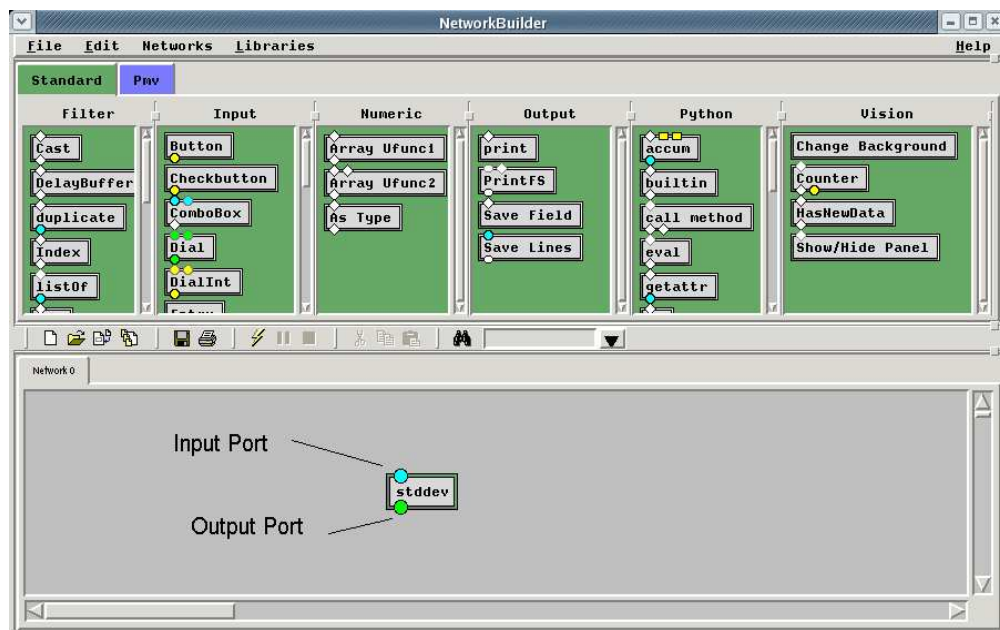
Vision **node** is a computational unit which takes input from **input port**(s), carries out the computation and output data to **output ports**. The outputs can be feed into other nodes for other computations. The connected nodes form a **network**.

Exercise 2: Load a simple Vision network.
1) click on 📂 icon and load the network "lena_net.py"
2) move the mouse pointer to the output port of "Read Image" node
3) press and hold middle button to move a node to new position.
4) double click the "Scale" node. Try to change the scale value with left mouse button. (click and move the pointer as if dialing an old fashion phone). Note the image size is changed.
5) try to click the "…" button on "Read Image" node and load another image: Groel4000_crip.jpg
6) close this network. ("File"->"Close")

Exercise 3: Construct a Polio varus capsid.
1) load "2plv.pdb" to PMV ("File"->"Read Molecule" or use the Dashboard),
   color this molecule by chain (click the "Chain" diamond on the Dashboard.
2) in Vision, "Libraries"->"Load Library"->"symlib"
3) drag-and-drop the following three nodes to the network editor:
   "Icosahedral" in "SymServer" library, "Macros" catalog
   "2plv" in "Pmv" library, "Molecules" catalog
   "Set Instances" in "Pmv" library, "Mapper" catalog
NOTE: you can always press and hold middle button to move a node to new position.
Now the screen should look this:
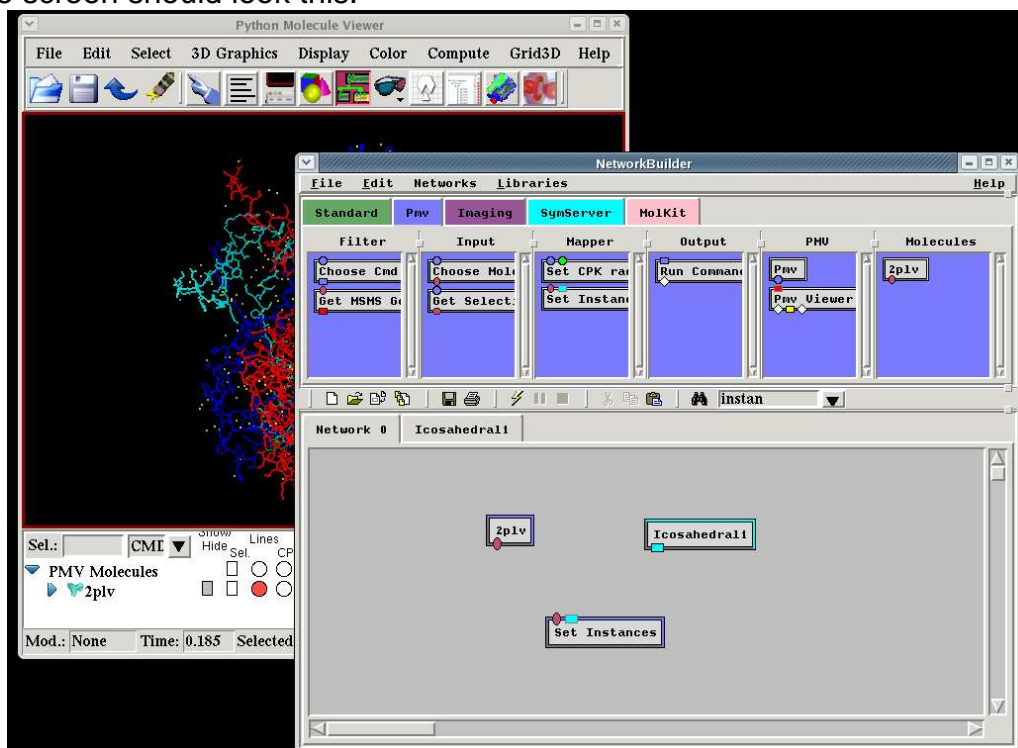
4) use the left button to connect the output port of "2plv" to the corresponding input port of "Set Instances". Make sure to match the color and shape of the ports.
5) connect the output port of "Icosahedral" to "Set Instances".
6) Now a network is built. To run it, click ⚡ button.
NOTE: click on the PMV window and press the key "N" to normalize: everything fits in the window.
NOTE: press the key "C" to set the rotation center at the center of all molecules.
NOTE: you can save this network by clicking 💾 .

Advanced exercise:
A1) move the mouse pointer over the connection between "Icosahedral" and "Set Instances", right click and choose "delete"
A2) double click the "Icosahedral" node to see know the transformation matrices are constructed.
A3) drag and drop "Translate" node from SymServer library, Transformations catalog. Double click this node and change the "vector length" to be 100.0 (one can either use the left mouse pointer to turn the thumb wheel, or right click the wheel ->Options. Type 100 as the Value input and click OK.
A4) send the output of "Translate" as input of "5-fold"
A5) double click the "Input Ports" node or use the tab to return to your network. Connect the output port of "Icosahedral" and "Set Instances".
Do you see the differences between with and without translation?

NOTE: Please close this Vision network and delete the 2plv molecule before going to the next exercise. (right click the 2plv label on the PMV Dashboard, choose "delete")

Application: Fitting GroEL structure to a EM map

Exercise 4: visualize a 3D Grid in PMV
1) click 🟥 icon on the PMV toolbar to open the control panel
2) click ➕ to load a 3D grid map
3) choose emd_1080.mrc
4) click on "Isocontour" icon to show histogram of the grid map (this may take a few seconds as the histogram of values is being computed)
5) shift-click inside the widget to add isocontour. This should create a bar inside the histogram and corresponding isocontour in the PMV viewer. Move this bar to change the isovalue. Let's try to set the isovalue to be 0.5
To rotate the surface: press and hold middle button
5.1) to change color of the surface, right click the bar, click "color"
5.2) to display the surface as mesh: right click the bar and choose "Set 3D surface properties". The "DejaVu GUI" should show up. Now click the "Front" button and set the value to be "line". Set the "Line Width" to be 0.10

6) click the "OrthoSlice" icon to display orthogonal slicing planes. Choose one or several directions and move the slider to see the planes.

7) hide the control panel by clicking .

Exercise 5: Fitting crystal structure of GroEL to EM map
1) load the crystal structure of GroEL ("File" -> "Read Molecule", choose 1OEL_A.pdb)
2) display secondary structure: click "Rib" on the Dashboard.
3) hide the line representation: click "Lines" on the Dashboard
4) color by secondary structure types: click "Sec Str" on the Dashboard
5) in Vision interface, load the network "demo_net.py" and run it. Double click the symmetry operation nodes such as "Translate", "Rotate", "2-fold" and "N-fold" to see how we adjusted parameters to fit the crystal structure to this EM map.

Be careful if you want to change the parameters. Every time a value is modified, the new transformation matrices will be updated and applied. This may lead to many redraw events (and therefore slow down your computer). To prevent this, please first freeze the network (by "Network"-> "Freeze Execution") first, after changing the values, uncheck the "Freeze Execution" and run the network.

A quick wrap-up
- The PMV-Vision architecture is built of Python modules. It was designed to open for new add-ons.
- The 3D Grid Rendering module in PMV can help EM users. Some other exciting features such as Volume rendering, plotting signature are under active development.
- Vision networks can be constructed with little programming experience and meant to be shared among users.