MolSlicer – A Tool For Removing Sections Of mol2mel Molecules

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MolSlicer is a program written in MEL script, which is made to be used in conjunction with mol2mel. Mol2mel is a program written by Benjamin Grosser that takes a Cerius .mol file and converts it into an Alias|Wavefront’s Maya .mel file. Once the molecule is loaded into Maya, molSlicer can be run to remove pieces of the molecule. For the time being, molSlicer can only do one slice per molecule. This may be changed on future versions.

Running Maya:

Maya is currently installed on Pollock, Hofmann and Arbus in the VMIL. To start the program, go to Start Menu -> Quickfind -> Maya. Once the program is running, you will need to do some initial setup.
First Time Users:

You will first need to create a project. A project is a place to store all of your files in order to avoid mess and confusion. To make a new project go to File -> Project -> New. In the box that opens click the Use Defaults button at the bottom. Then enter your username as the project name on top and set the project path to a folder on drive H, which is your home directory on the network. DO NOT use the default path as your project path. This path will store your work in your profile and can make it take a VERY long time to log in and out of the computers. Once this is done click the Accept button.

Opening molSlicer
Look on the second row of icons near the top of the Maya window. There should be an icon which looks like a meat cleaver. If you do not see this, hold down the right mouse button over the folder icon at the beginning of this row and select ITG. This will set the shelf to the ITG shelf. You should now see the icon. Click on the icon to begin the script.
Intersection vs. Difference

When you run the molSicer script from the shelf, this window will open and a cube will be created on the screen. The number of points in the cube will be different depending on which version of the script you ran. There are 3 choices on how to slice the molecule. The first choice, difference, will cut out any piece of the molecule that overlaps with the cube shape. Intersection does the opposite. It will get rid of any part of the molecule that does not overlap the cube, only keeping the part of the molecule inside the cube shape. To gain more speed when running the intersection option, you can choose intersection fast. This only works if you are taking a complete slice through the molecule. It speeds up the process by only analyzing and slicing the atoms on the border of the cube, disregarding anything in the middle. If you are not doing a complete cut, or are using a complex shape, the intersection (slow) option should be used. This will analyze all atoms including the ones not on the borders.

Moving around in Maya

Moving around in Maya can be done with a few simple combinations. First, whenever you wish to move you must hold down the alt key on the keyboard. With the alt key depressed, you can then move around with the mouse. The combinations are as follows:

Orbit -> alt + left mouse button
Pan -> alt + middle mouse button
Zoom -> alt + left and middle mouse button

Manipulating Points of the Cube

There are several techniques that can be used to size and shape the cube. First, you should treat the cube as an object and get it to the approximate size.
In the first row of icons under the main pull down windows you can see the object selection button recessed. This means you are manipulating the cube as an object. On the next row down there are six large icons starting on the left. In this window the selection icon is selected. These are the tools you will use to manipulate the shape. Next to the arrow-shaped selection icon is the move tool, followed by the rotate and scale tool. These are the only tools you will need to resize and reshape the cube. First click on the cube, then select the tool. The tool will have three axis on it allowing you to move, scale and rotate on the x, y or z axis. To do this, just left-click on the tool axis you wish to adjust and drag the mouse. This will allow you to scale the cube to the right size, and rotate and move it into the proper orientation.

If you would like to reshape the cube to a more complex shape than can be made with the basic 8 point cube, you can add more points to it. With the cube selected, look on the far right side of the screen in the Channel Box. About half way down you should see the word INPUTS with polyCube1 underneath it. Click on the work polyCube1. You should now see settings for subdivisions of width, height and depth. You can change these numbers to whatever you would like. It is recommended to use the fewest number of points possible which will still allow you to get the shape you desire.

To reshape the cube, you will need to first select the cube in object selection mode, then choose the select by component button and choose points as the pick mask. This looks like this:

![Select by Component](image)

The points on the cube will now be visible. You can now select only the points you wish to manipulate and use the move, rotate and scale tools to adjust the shape of the cube to whatever you desire. Here is an example of the molSlicerComplex cube adjusted to a particular shape:
Once the cube is adjusted to your satisfaction and positioned correctly in the molecule, you are ready to perform the slicing operation.

**Slicing the Molecule**

To slice the molecule, select the molSlicer interface window, then select the radio button for the type of operation you desire; difference, intersection (fast) or intersection (slow). If you would like a progress report to view the progress on the molecule, you should now open the script editor. To do this, use the pull down menus at the very top of the screen. Select `Window->General Editors-> Script Editor`. Drag the corner of this window to resize it if you with. Then, when ready, click the complete button in the molSlicer interface window and the operations will begin. Once all the atoms have been analyzed, the script editor will tell you it is done by printing the text, "End of all elements." You now have the sliced molecule.

**Assigning Priority to Shaders**

If you have a molecule with multiple types of atoms, you may need to assign priority to shaders. You will only need to do this if your cut goes through different atoms that are overlapping. Where two different atoms overlap on the cut, there will be common space with two shaders assigned which Maya does not know how to deal with. To fix this problem, a slight translation should be applied to the atoms which you would like to have priority. Select one of the overlapping groups, for example C_sliced or N_sliced, and figure out which axis to move them on. You should adjust them on the axis which is perpendicular to the plane of the cut. If that is the X-axis, go to the channel box on the right of the screen and add a value around 0.003 to the translate X field. This will move them off the plane slightly so Maya knows their shading group is over the other shading groups. You will need to do this for any overlapping groups until there are no overlapping shaders.
Error Messages in Script Editor:

For some of the atoms it will print an error message in the script editor saying to move the atoms slightly. This should be ignored. They way the molSlicer works is by analyzing the bounding box of the entire cube. This is another large cube that fully encloses the cube shape you have made. If you have part of the cube scaled down, for example, a wedge, all atoms in the bounding box will still be processed, even if at that particular point the cube is scaled in and doesn’t actually intersect with the atom. When this occurs that error message will show up. It has no effect on the cutting process and should just be ignored. This error is used as a buffer to allow you to completely change the cube shape and still receive the desired cutting of the molecule.

If you have any questions or problems with this script, please email jrgilles@itg.uiuc.edu and we can set up a time to get together.