Week-05 Homework
Introduction to Visit and Datasets

In this homework, you will work with 3 data files that are in the zipped data files found on D2L. Unzip the folder to a location that will be easy for you to work with.

If you prefer to work on the visualization cluster using EnginFrame and the Visit 2.10.0 module, please feel free to transfer your files up to your /home or /projects directory and work from there. After you have completed your work, you will need to transfer your images back to your local machine to prepare your report.

You will be asked a series of questions regarding the data and then to create a .png file of a very simple visualization for the dataset. You will prepare a report with your answers to the questions and a copy of the image imbedded in the report. Save your file as a pdf file (yes, pdf file is just fine, anything else not so fine, as in don't) and upload it to the D2L dropbox.

Carefully read all the directions. While some look similar to previous directions, they may actually be different!

Please note that there are differences in the gui between Windows and MacOS versions of Visit. Where we know there is a difference the MacOS equivalent is in brackets '[]'.

Initial Visit setup

- In the main VisIt 2.10.0 control panel under the 'Global' section make sure 'Auto apply' is checked.
- From the 'Options' menu, select 'Host Profiles' ['Host profiles …'] and set 'Username' to your first and last name. 'Apply' and 'Dismiss'
- From the 'File' menu select 'Set save options' ['Set Save options'] and set the following options:
    - Define a 'Filename' for your files you will be saving.
    - Set Output directory to where you want to save the files to.
    - Set 'File type' to png'
    - Set 'Aspect ratio' ['Resolution'] to 'Screen ratio'
    - Set Width to 800
    - 'Apply' and 'Dismiss'
- From the 'Options' menu, select 'Rendering …'
    - Under the 'Basic' tab make sure 'Antialiasing' is checked.
- From the 'Advanced' tab set the following options.
    - 'Use scalable rendering' = 'Auto'
    - 'Shadows' = unchecked
    - 'Depth cueing' = unchecked

Click on the 'Open' button in the 'Sources' section and set the path where you stored your data files. Turn on the checkbox for 'Use "current working directory" by default'.

Dataset 1: strpts3d.vtk

Open the strpts3d.vtk file, and using the 'File Information' identify the following information:

- **Data File Name:**
- **File Format:**
- **Mesh Type:**
- **Spatial Dimensions:**
- **Spatial extents:**
- **Names of Scalars:**
- **Names of Vectors:**
- **Names of Expressions:**

In the 'Plots' section, add the following plot attribute: Pseudocolor->Temperature

Rotate the object so the z-axis (on the object itself) is pointing down toward the bottom-left corner of the window, the y-axis is pointing up towards the top-left of the window, and the x-axis is on the right side of the window.

Move the object so that it is not intersecting with the color bar.

Expand the Plot attribute by clicking on the arrow and double click on 'Pseudocolor' and set the following options

- 'Color table' = 'hot'
- 'Opacity' = 'Constant'
- Move the Opacity bar to 50%
- 'Apply' and 'Dismiss'

Under the 'Controls' menu, select 'Annotation'

- On the 'General' tab make sure the following checkboxes are checked, 'Legend', 'Database','Time', 'User information', 'Use foreground color'
- On the '3D' tab check 'Show axes', 'Show triad', and 'Show bounding box'

Using the either the File->Save window option or ctrl+s [command-s] to save your rendering.

'Delete' your plot attribute and 'Close' the source file.

DATA SET 2: global_node.silo

Open the global_node.silo file and using the 'File Information' provide the following information:

- **Data File Name:**
- **File Format:**
- **Mesh Type:**
- **Spatial Dimensions:**
- **Names of Scalars:**

Add the following plot attribute: Mesh->mesh

Expand the mesh attribute, double click on 'Mesh' and set the following options:

- 'Show internal zones' = checked
- 'Mesh color' = 'Custom', set the color to a darkish blue.
- Opaque mode = Off
- Opacity = 20%

Rotate the object so the z-axis (on the object itself) is pointing down towards the bottom-left corner of the window, the y-axis is pointing up towards the top-left of the window and the x-axis is around half way up the right side of the window.

Under the 'Controls' menu, select 'Annotation'

- On the 'General' tab make sure the following checkboxes are checked, 'Legend', 'Database','Time', 'User information', 'Use foreground color'
- On the '3D' tab check 'Show axes', 'Show triad', and 'Show bounding box'

Save your rendering using File->Save window or ctrl+s [command+s]

'Delete' your plot attribute and 'Close' the source file.

DATA SET 3: 1b41.pdb

Open the 1b41.pdb file and using the 'File Information' provide the following information:

- **Data File Name:**
- **Data Description ('Database comment'):**
- **File Format:**
- **Mesh Type:**
- **Spatial Dimensions:**

Add the following plot attribute: Molecule->element

- Expand the attribute and double click on 'Molecule'
  - From the 'Atoms' tab set the following;
    - 'Draw atoms as' = 'spheres'
    - 'Atom sphere quality' = 'Super'
    - 'Radius based on' = 'Atomic radius'
    - 'Atom radius scale factor' = 1.25
    - From the 'Colors' tab, set 'Element types' = 'cpk_jmol'

Under the 'Controls' menu, select 'Annotation'

- On the 'General' tab make sure the following checkboxes are checked, 'Legend', 'Database','Time', 'User information', 'Use foreground color'
- On the '3D' tab uncheck 'Show axes' and 'Show bounding box' – leave 'Show triad' checked

Click on the 'Objects' tab

- Click on 'Text' and enter 'Title' when asked 'Enter a name for a new annotation object.' Click 'OK'
- For 'Text' change '2D text annotation' to 'Human Acetylcholinesterase'.
- Click on the 'Bold' check box.
- Left click on the arrow to the far right of 'Lower Left' and with the button still down move the cross lines to position the title in the top center. Alternatively, you can use the numeric text box (try starting with 0.4 0.94)

Feel free to move your object around to look at it. When done right click in the rendering window and from the hot-key menu select View->Reset view.

Using the either the File->Save window option or ctrl+s [command+s] to save your rendering.

Delete your plot attribute and 'Close' the source file.