3D Carboxysome Visualization with ThreeJS

Tuesday, November 05, 2024   3:24 PM

- **Introduction**

This script utilizes Three.js, a JavaScript library to display animated 3D computer graphics in a web browser using WebGL, to display a simplified 3-dimensional model of a Carboxysome and visualize the Rubisco within it. It is intended to run with a cleaned and sub-tomogram averaged Dynamo table ('.tbl') as input. That is, the script will model the proteins as originally read from the tomogram, as opposed to modeling the chain output obtained after running the data through our polymerization scripts. By modeling the unprocessed tomogram data we obtain a reference of what the microcompartment really looks like and we can use it for comparisons and to test the output of the scripts. It will also allow us to visualize if there are any problems with the dataset or if it was not properly cleaned and polished.

- **Usage Instructions**

This script and the necessary files to run it are available in the following path:
/net/metskas/shared-scratch/vfenton/Visualize_Carboxysome_3D

To run this script, simply 'cd' into the specified directory, and run the command '**npx vite**' to host a local website where the model will be displayed for use. In the Metskas Lab workstations, all the necessary modules and environments are already installed, so no additional steps should be required.

-> If you are attempting to run this script externally, you must ensure that the following environments and modules are installed on your machine and up to date: Node.js -- Three.js, Vite.js, Dat.GUI.

If successful, you will see a response as the above where vite is hosting a website on an available port of your machine's localhost. Then simply 'ctrl + click' or copy and paste the provided URL into your browser

- **User Input**

When first loading the website, you'll be met with user input dialogs to specify the input data file, the Carboxysome number to model within that file, and which Rubisco or Rubisco chains within that Carboxysome you wish to highlight, if any.

1. Input File:
The input file must be a Dynamo table (a file with extension '.tbl' and following the tomography Dynamo format) **within the same directory as the Visualization script**. That is, the input file must also be in 'Visualize_Carboxysome_3D/'. Since the scripts are in my shared-scratch directory, you will not be able to copy or move any files into the directory. There are currently 3 sample files in the directory, which correspond to the current (as of 11/07/2024) Rubisco data we have for DTT, diamide, or wildType/untreated treatments. However, **if you wish to run this script on updated data or a different dataset, you will have to copy the entire directory into a folder where you have write permissions (your scratch folder), copy the desired dataset inside of the directory, and run it from there.** Once a file is in the same directory as the visualization script, you may use it simply by entering the file name in the prompt.
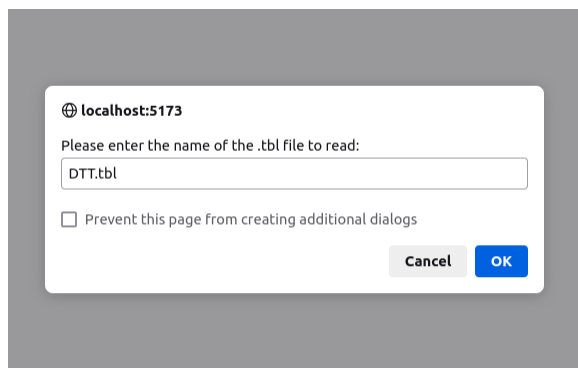
2. Carboxysome number:
   Enter the Carboxysome number or ID (column 21 of the dataset) which you wish to visualize.

3. Tags to Highlight:
   In the third prompt, you may enter specific rubisco or chains that you want to highlight by specifying their tags. If you wish to highlight or mark specific individual rubisco, enter a list of their tags, e.g. [764, 563, 566]. Ensure that the tags you are entering correspond to the Carboxysome number specified in the second prompt, or else nothing will be highlighted. If you wish to highlight chains of rubisco, enter a list of tag lists, e.g. [[691, 714], [616, 630, 639, 708], [703, 533], [702, 610]]. In the 'Random' color setting, rubiscos within a particular chain will all have the same color, but the colors across different chains will be randomized. If you do not wish to highlight any rubisco and just want to look at all of them equally, simply hit enter or click the 'Cancel' button on the browser prompt.

- **Main View**

Once all user inputs have been entered (and if all the information entered was valid), the following view will be rendered:
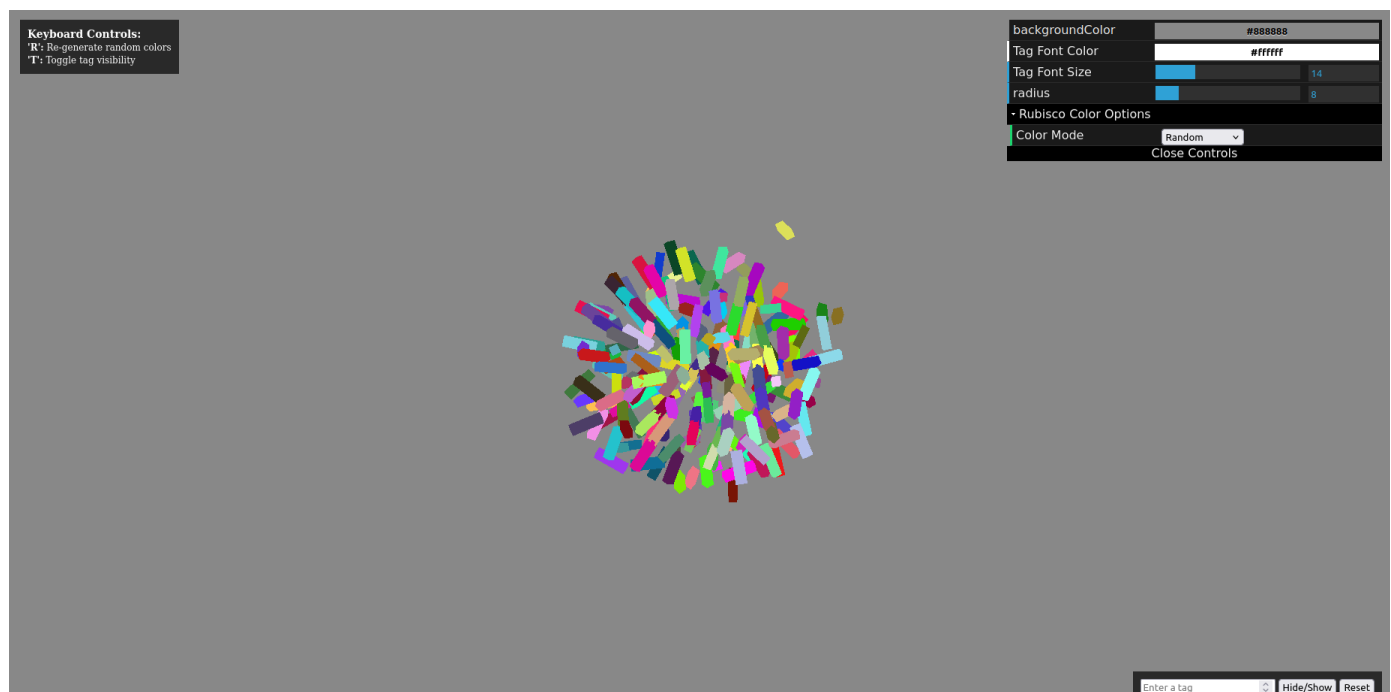
*Developer Note: If an error occurs or something is not displaying or not working properly, inspect the page (ctrl + shift + i) and check the console output for any error messages to debug.

The User controls are pretty self-explanatory and all displayed in overlays in the screen corners.

- Use the mouse to navigate the model. You may rotate around the model by clicking and dragging with the left click. You may transpose/move the model by clicking and dragging with the right click. You may zoom in and out of the model by using the scroll wheel.
- Hitting the 'r' key will re-generate the random colors (if in Random color mode).
- Hitting the 't' key will toggle (show/hide) the tag numbers of all rubisco objects shown.
- The user controls in the top right corner include sliders, color pickers, and dropdowns to modify parameters such as the background color, font color, font size, rubisco object radius, opacity of unmarked rubisco, color mode, uniform color, etc.
- The dialog in the bottom right corner allows the user to Hide specific Rubisco in the model by typing in the tag number of the Rubisco to hide and hitting enter or clicking the 'Hide/Show' button. A list of hidden tags will be updated to show all rubisco that are hidden. If you wish to bring back or show a hidden rubisco, simply type its tag into the input box and hit enter or click the button again. To show all rubisco again, you may click the 'Reset' button.

Enter a tag   Hide/Show   Reset
Hidden Tags: 3969, 3992, 3927, 3993