

Two Alternative Methods of Creating Molecular Surface Models

1. Using electron microscopy (EM) data from the Electron Microscopy Data Bank (EMDB)
2. Creating a Coarse Metaball Surface per Chain for Multi-Subunit Molecules

Creating an Ebola Virus Spike Model from EM Data

Ebola Spike CryoEM Structure File:

- > EMD-6003 (emd_6003.map)
- > emd_6003.map can be downloaded from the Electron Microscopy Data Bank (EMDB): http://emsearch.rutgers.edu/atlas/6003_downloads.html

Download EMD-6003 and uncompress.

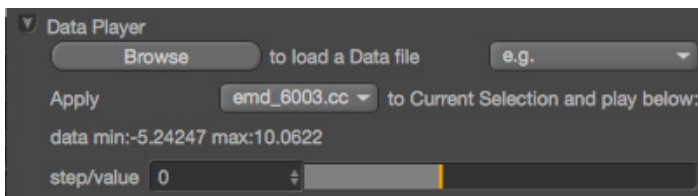
Windows users may need to install an unzipping freeware package

Change the name of the downloaded file's .map file extension to .ccp4 so the precise file is named emd_6003.ccp4

Start a fresh ePMV session (Open Cinema4d & ePMV)

Generate a Cinema4D object from EM map

ePMV > Unfold Data Player



Browse and load the emd_6003.ccp4 file

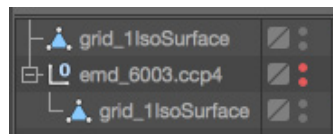
This may take a minute with larger EM files than this.

Click the "Apply [option] to Current Select and play below:" dropdown and reselect emd_6003 to initiate the data slider

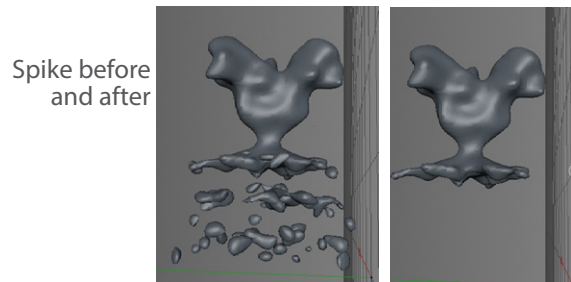
Change 0 to 1 and hit return to get a good mesh.

EM maps are volumetric data, and the data slider determines the threshold that is being used to translate the volumetric data into the surface representation that you see on your screen. Try a few different values to get a sense for this variation within the dataset.

Make a copy of grid_1isoSurface and remove it from the emd_6003.ccp4 hierarchy. Hide the emd_6003.ccp4 hierarchy.



Remove residual noise from around the spike copy. (Use point-edit mode to select and delete the vertices you want to remove).



Rename the object "Clean Spike"

Re-center the axis of Clean Spike (Mesh > Axis Center > Center Axis To)

Set Clean Spike coordinates to 0, 0, 0.

Toggle "Enable Axis" icon.

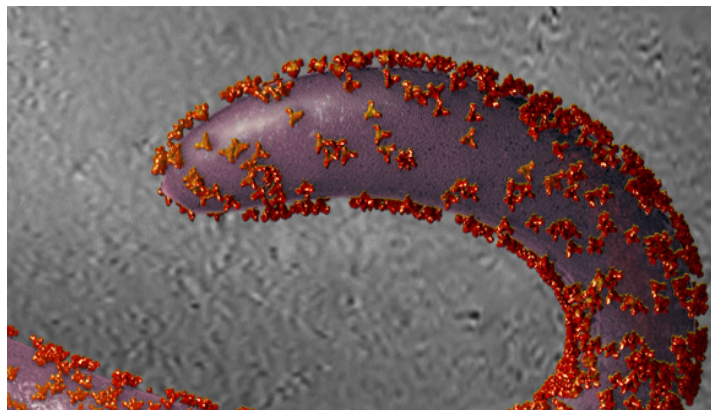
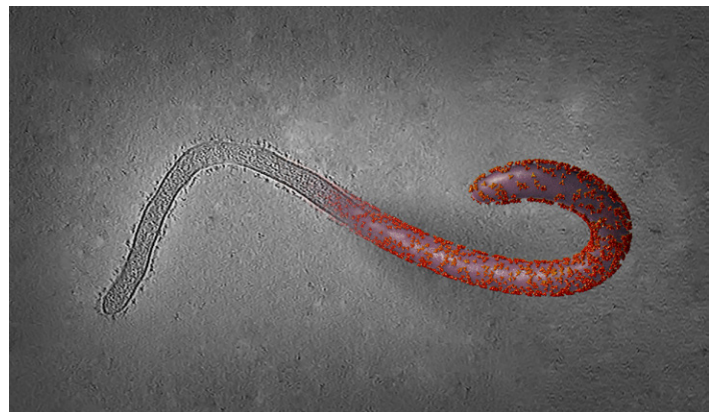


Set the axis of the Clean Spike to be near the bottom, where it intersects the membrane.

(If you want, rotate the axis in this mode so that the Y-axis (green) is along the vertical axis of the spike.

Otherwise you will need to set the rotation in the cloner)

The EM data derived spike object is now ready to be cloned onto a virus shape!



Creating a Coarse Metaball Surface Per Chain for MultiSubunit Molecules

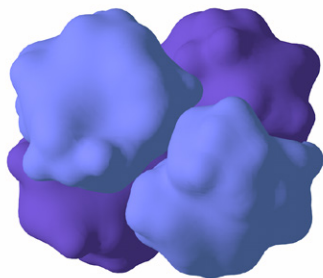
Start a fresh ePMV session

ePMV > Edit > ePMV Preferences >

- >Change Default representation to "None".
- >Click [Apply and Close]

Fetch PDB 1hho (hemoglobin).

(This fetches the dimer of hemoglobin, which works for this example, but you may want to create the biological unit, a tetramer, shown here)



Create a spline backbone

- >Backbone representations > Check [✓] spline

Create a Single Point object

- >Create a new polygon object.
- >Make editable (Shortcut "C")
- >Delete all but one point in point edit mode.
- >Re-center the axis to the remaining point.
- >Rename Polygon object "Point"

Create a cloner and make Point a child of the cloner.

Set the cloner as follows:

- >Mode: Object
- >Object: 1hho_Aspline (Find this in the hierarchy under 1hho > 1hho:A)
- >Distribution: Step
- >Step: 11

Now we have points cloned along the length of the backbone spline for the A-chain of hemoglobin.

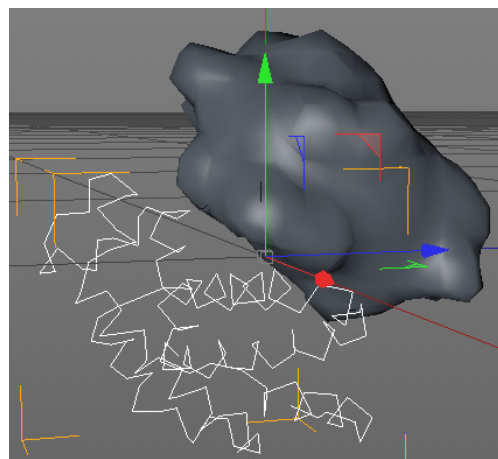
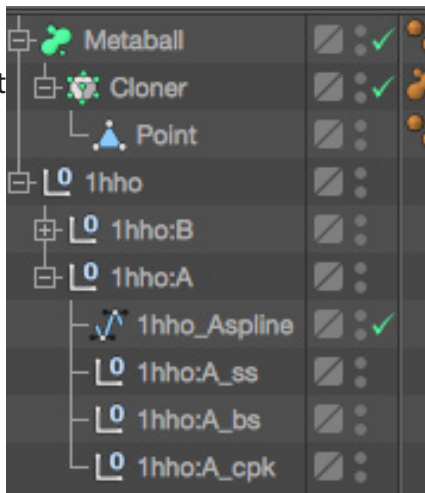
Create a Metaball object and make the cloner a child.

Add a Metaball Tag to your cloner object (Tags > Cinema4D > Metaball)

Metaball Tag

- >Radius: 2
- >Metaball:
- >Editor
- Subdivision: 3
- >Render
- Subdivision: 1

(These are just some suggested starting values. Adjust Metaball, tag, and cloner settings as you like to get a result that you like)

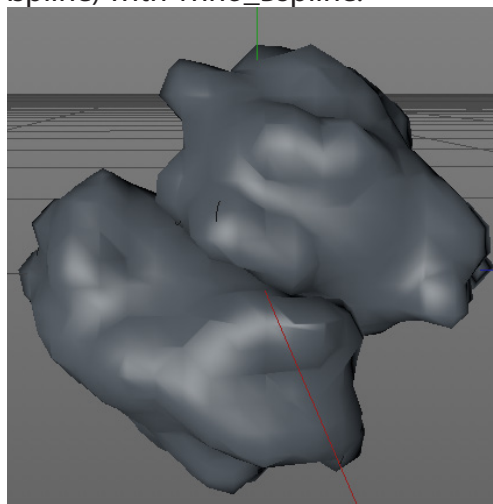


Once you have Metaball settings you are happy with, rename your Metaball "Surface Chain A"

Duplicate Surface Chain A.

Rename the duplicate "Surface Chain B".

Replace Surface Chain B's Cloner object (currently 1hho_Aspline) with 1hho_Bspline.



Now we have a coarse Metaball surface for each chain of the protein! For an easy way to manage your multiple Metaball objects all in one place, see the Xpresso handout.