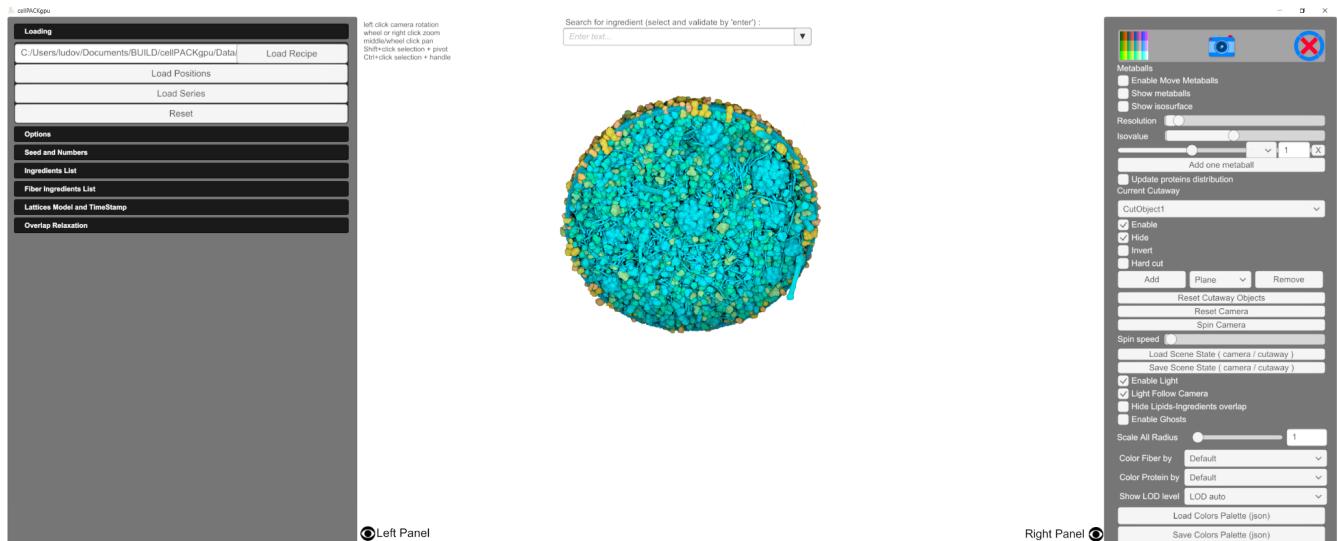


Modelling Mycoplasma Genitalium in cellPACKgpu

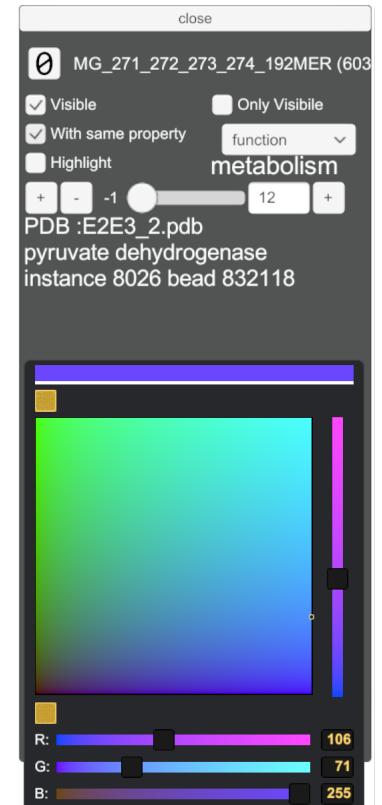
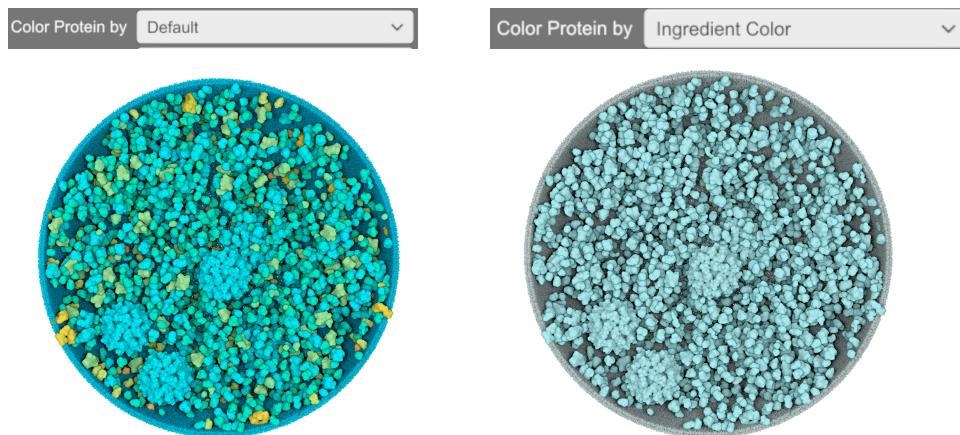
After starting cellPACKgpu.exe you should see by default the model built for the curated recipe and the frame 149 from the whole cell simulation. The scene is clipped with a plane placed at the center of the cell. The color is the default automatic coloring per compartment. The ingredient defined color is based on the function categories.



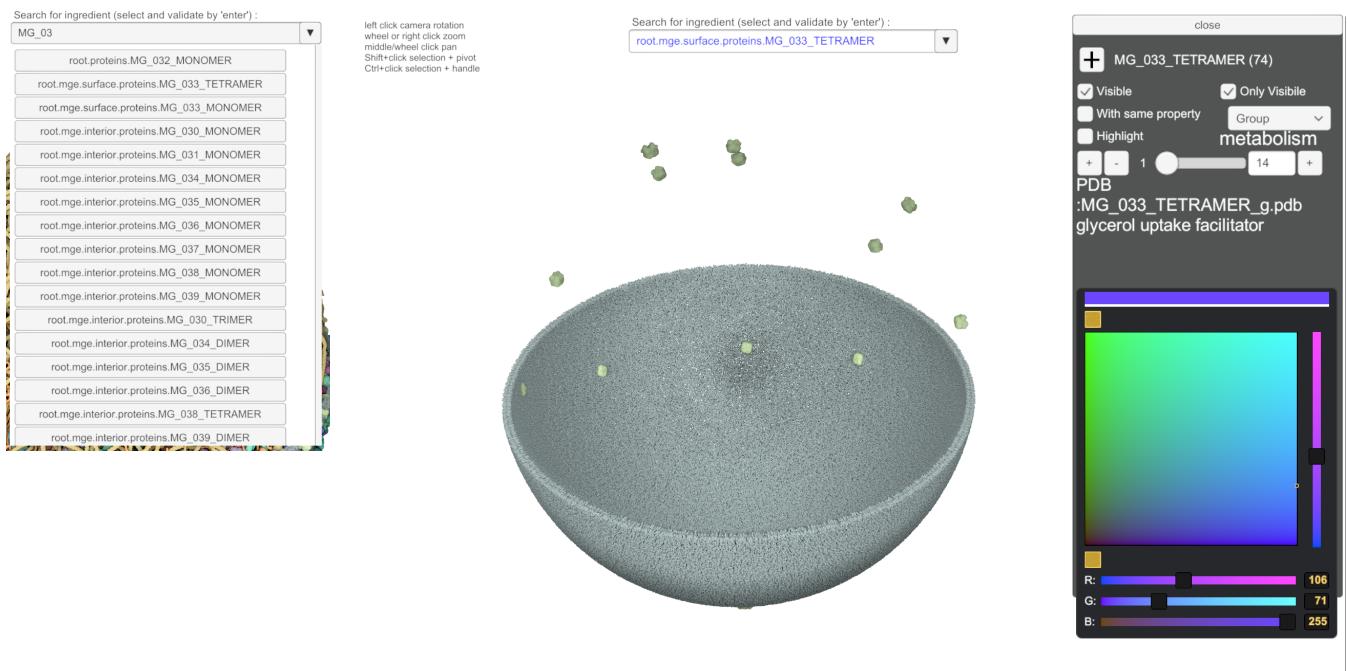
[Have a look at the User Interface quick description](#)

1- Exploring the model

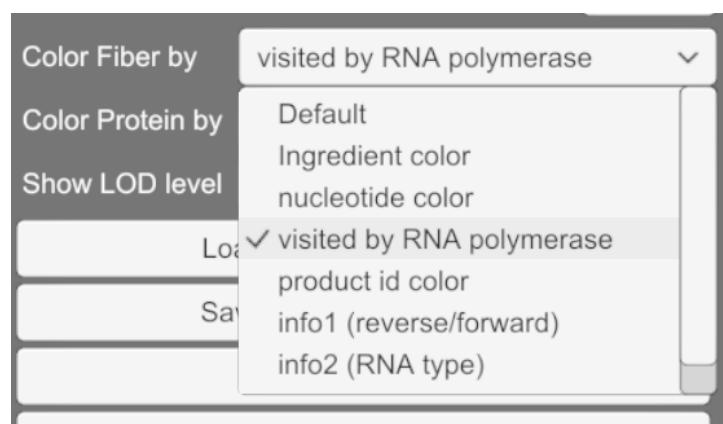
You can explore the model by looking at the individual protein by selecting them e.g. **ctrl+left-click** this will pop-up the Ingredient panel. It will tell you the name, the PDB file associated and a description of the selected molecule. This panel give you different options in terms of visibility. Next to the name there is a three state toggle that changes the clipping states (-1 completely invisible, 0 cut by the current cutaway object, +1 not cut by the current cutaway object). You can completely hide all instances of the molecule with the “visible” toggle. Or you can hide everything else using the “Only visible” toggle. The “With same property” will make only visible the current molecule and any molecule that share the same selected property. In the adjacent image, we choose to show only the molecules with the same function (here “metabolism”).



If you don't visually find a given molecule, you can use the search bar and provide a name. The search bar is case-sensitive and every molecule name in the whole cell simulation data is upper case and based on the gene name. Below is an example: after typing 'MG_03', the panel will show you all molecules with a name starting with MG_03. We then picked MG_033_TETRAMER, click in the field and type enter. This will select the molecule. Then clicking "Only visible" will show only all instance of that given molecule.



For this particular release we have added more coloring schemes for the nucleic acid (DNA and RNA).



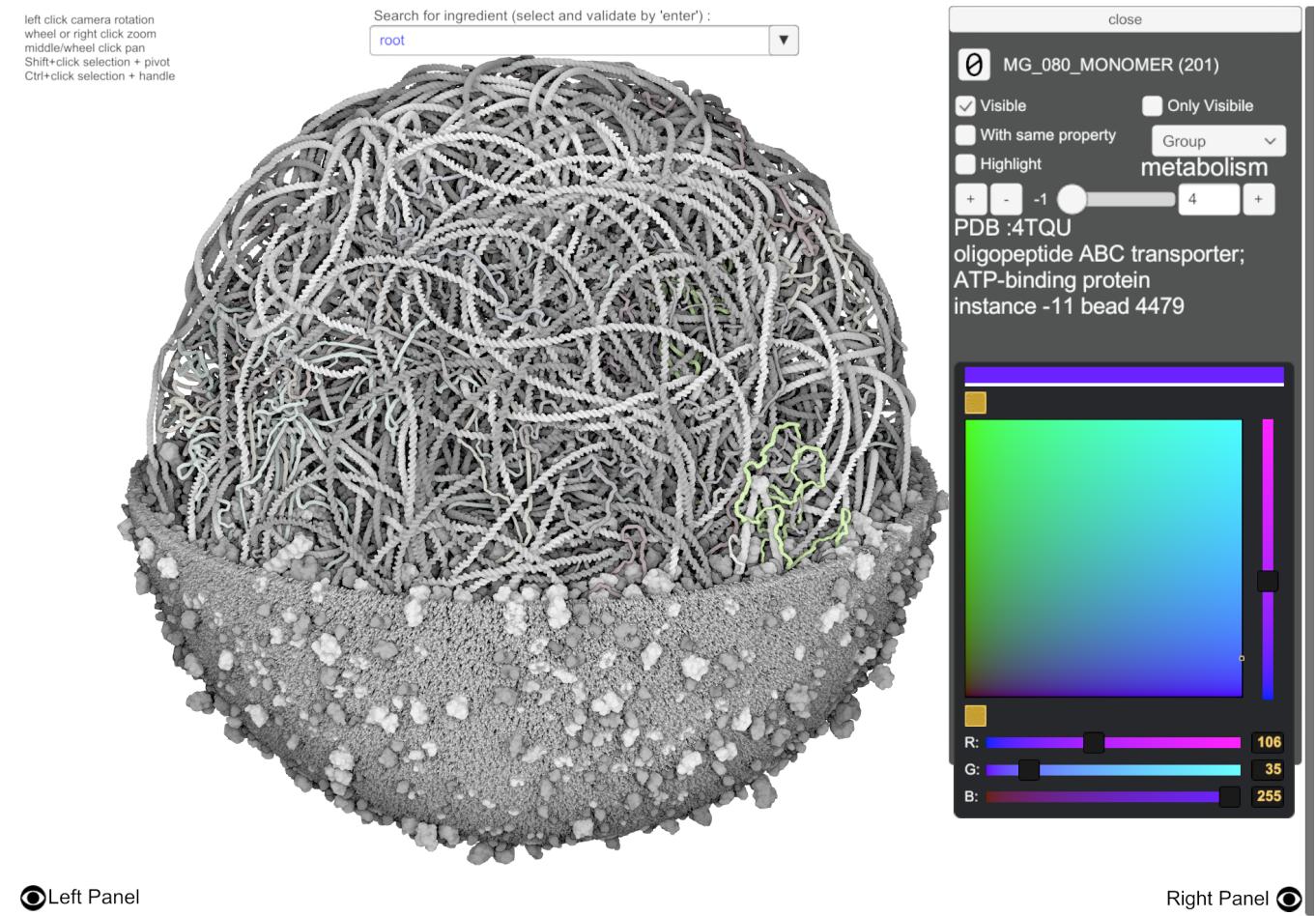
- Default use the automatic color assignation based on compartment
- Ingredient color use the color define in the recipe (here generated in mesoscope based on the ingredient function)
- Nucleotide color use a color per base pair
- Visited by RNA polymerase for the given frame, use two color : one for visited and another for unvisited
- Product id color: use the color of the protein that the gene is coding for.

- Color by the sens of the gene
- Color by the type of RNA this gene code for (mRNA, rRNA, etc...)

Note that any of this color can be changed using the color widget and then save/load.

Load Colors Palette (json)
Save Colors Palette (json)

When using the color fiber by product id color, the selection system changes for the fiber. If you ctrl+left click on the RNA or DNA it will who in the Ingredient panel the protein for which they code for. Below is an example with the mRNA encoding for MG_080_MONOMER highlighted.



2- Cutaway Objects

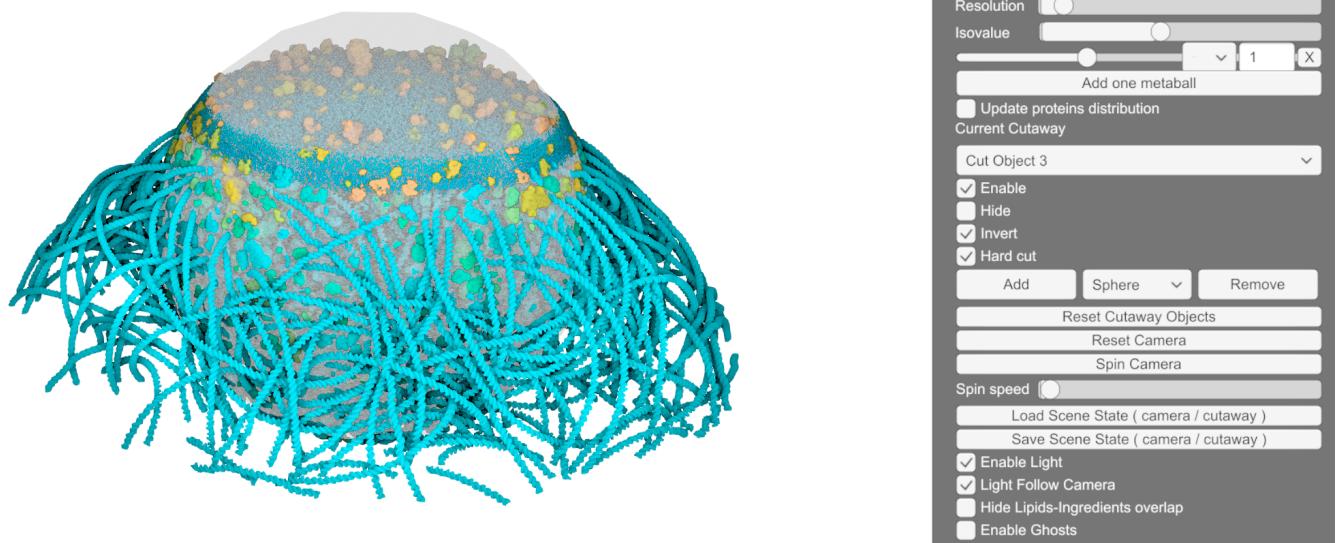


At start there is always a cutaway plane object. You can control all the clipping options from the right panel. All the toggle buttons will apply to the current selected cutaway object from the pull down menu.

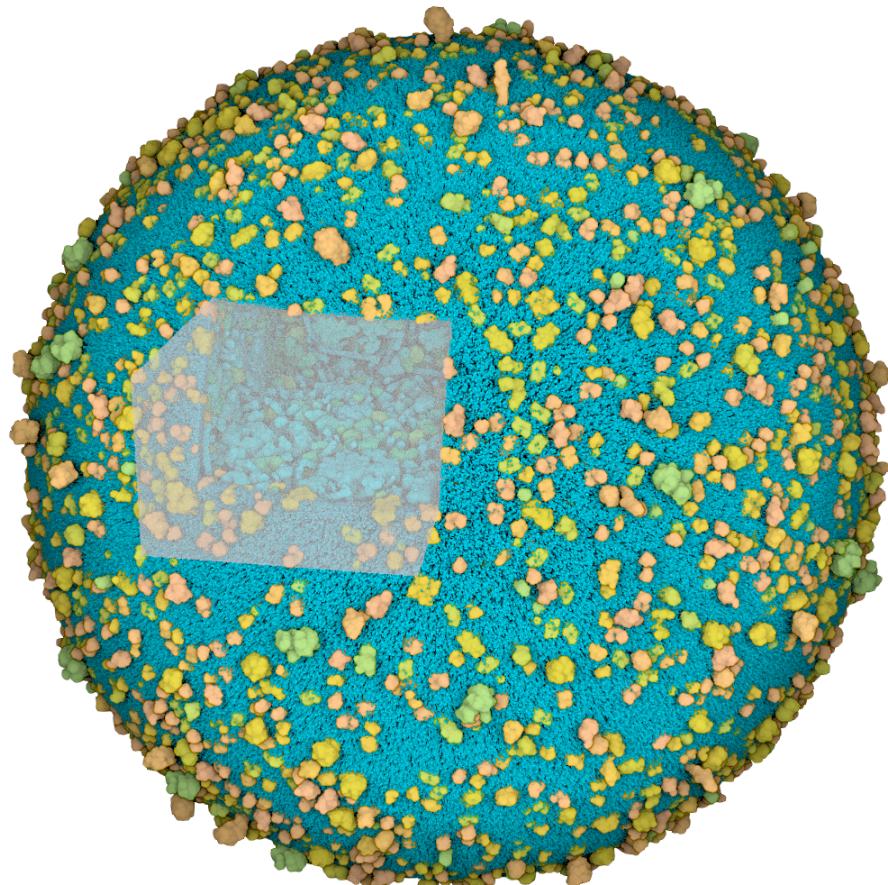
The hard-cut option will cut at the atom/bead level, while the default will cut at the molecule level. When enabled you can unhide it to make it visible and selectable. You can select the object with ctrl+left-click. The transform handle will appear to

let you interactively move it. To rotate it or scale it you can change the handle type using the keyboard keys : 1-translate, 2-rotate, 3-scale. Once selected you can also change the type.

Below as an example, we change the plane to a sphere and invert it to cut away outside the sphere. We excluded the DNA for being affected by it and we added a plane cutaway to affect everything.



Another example with a visible cube cutaway, with hardcut mode.



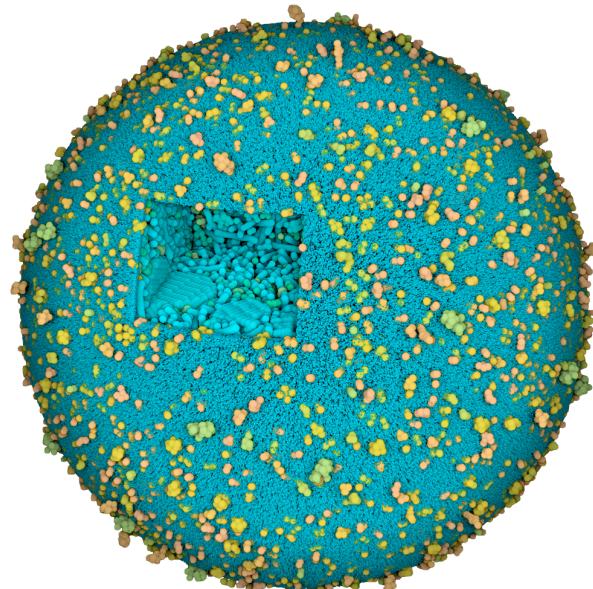
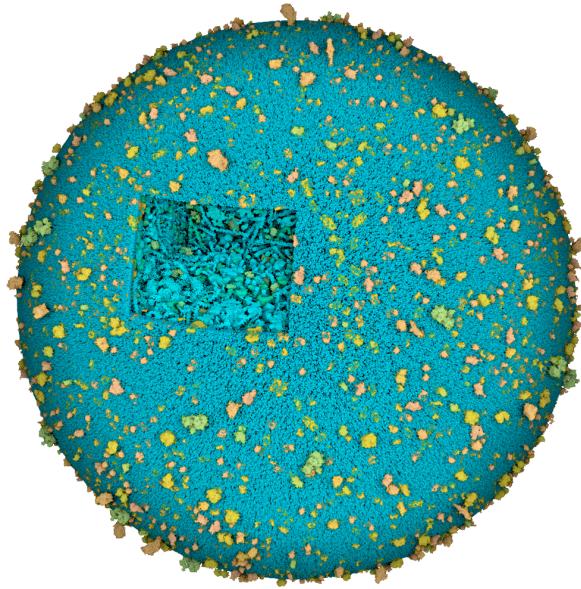
2- Level of Details

cellPACKgpu is built on top of cellVIEW which uses dynamic LOD with the camera distance. However we provide a pulldown menu which can enforce one given level. Levels go from 0 (all atom), 1-2-3 (automatically build beads), 4-5 (defined in the recipe).

Scale All Radius	<input type="range" value="1"/>
Color Fiber by	Default
Color Protein by	Default
Show LOD level	LOD auto

Show LOD level

Show LOD level



3- Changing recipe and frame

At the start all the left panel sections collapsed. Click on the title to open/close each section. Click on LAttices Model and TimeStamp to open the special section for mycoplasma genitalium. You can load each of the three timestamps selected for this project. And you can switch to the alternate automatic recipe which only uses automatically assigned structure for every ingredient.

When switching between recipes, be patient as the application will reload all the different protein structures.

149/150
✓ 149/150
1184/1189
6973/6960

Curated
✓ Curated
Automatic

Loading	
C:/Users/ludov/Documents/BUILD/cellPACKgpu/Data/	Load Recipe
Load Positions	
Load Series	
Reset	
Options	
Seed and Numbers	
Ingredients List	
Fiber Ingredients List	
Lattices Model and TimeStamp	
Recipe	
Curated	Time Stamp (MONOMER/COMPLEX)
149/150	Calculate PL
Overlap Relaxation	

4-Creating a Model

4.1 Change the distribution

4.2 Relax

4.2.1 Gpu Relax

4.2.2 Flex Relax

4.3 Save the model

TROUBLESHOOTING

- If the viewport becomes black restart the app.
- If the app becomes unresponsive, force quit it.