

Left Panel

Loading

C:\Users\hudo\Documents\BUILD\PACKgpu\Del Load Recipe

Load Positions

Load Series

Reset

Options

☒ Update Voxelisation real-time

VSize

☐ Show Bounding Box

☐ Show Voxels

☐ Show Voxels Occupied

☐ Show Procedural Ingredients Mesh

☐ Show Compartments Mesh

☐ Populate Exterior Ingredients

☒ Populate Surface Ingredients

☒ Populate Lipids Surface

☒ Populate Interior Ingredients

☐ Grow Fiber

☒ Populate Procedural Ingredients

☐ Grow Fiber real-time

☐ Populate Spawning Ingredients

☐ Populate Spawning Fiber

☐ Visual Jitter

☐ Show all Ingredients on a 2D grid

Seed and Numbers

Set Random Seed

Enter Seed

reset to zero reset to current volume Load

Protein Number: 2854916

Time: 0.34

Ingredients List

Add one Ingredient

| Ingredient ID | Compartment ID | Count |
|---------------|----------------|-------|
| MG_032_MONO | 0 | 0 |
| MG_074_MONO | 0 | 0 |
| MG_096_MONO | 0 | 0 |
| MG_129_MONO | 0 | 0 |
| MG_146_MONO | 0 | 0 |
| MG_220_MONO | 0 | 0 |
| MG_286_MONO | 0 | 0 |
| MG_310_MONO | 0 | 0 |

Fiber Ingredients List

Add one Fiber Ingredient

| Ingredient ID | Compartment ID | Count |
|---------------|----------------|-------|
| DNA (0) | 0 | 0 |
| 100000 | 0.25 | 34 |
| RNA (1) | 1 | 0 |
| 2500 | 1.4 | 34 |
| peptides (2) | 2 | 0 |
| 200 | 2.09 | 10 |

Lattices Model and TimeStamp

Recipe

Curated

TimeStamp (MONOMER/COMPLEX)

148/150

Calculate PL

Overlap Relaxation

Run One Step Relaxation

☐ Continuously Run Relaxation

☐ Force Reinitialisation

Beads Level

DNA persistence

☐ Show Beads

☐ Show Clashes

Method

☒ GPU overlap ☐ Flex ☐ Flex Shared Memory

Scale Torque

Scale Force

☐ compartment overlap

☐ inside overlap

☐ Draw Flex Particles

☐ Draw Flex Springs

☐ Expand radius loop

Expand to Radius

Current Radius : 0.17

Damping

Gravity x

Gravity y

Gravity z

☒ Fix selection

Loading Panel :

- Load serialized recipe
- Load .bin model file that hold position and rotation of each molecules
- Load .traj or folder of .bin as a series
- Reset the current scene

Options Panel :

- Voxelization of the volume in real time and Voxel size
- Show volume bounding box
- Show the voxels as spheres, show only occupied voxel
- Distribute macromolecules in the exterior compartments
- Distribute macromolecules at the surface of the compartments
- Distribute macromolecules inside the compartments
- Distribute lipids tiles at the surface of the compartments
- Grow/Distribute Fibers
- Visual jitter : randomly move the macromolecules
- Show all ingredients on a 2D grid

Seed and Numbers Panel :

- Set the random seed for the distribution
- Reset all the copy number to 0
- Reset all the copy numbers based on the molarity and the compartment volume
- Load a molarity / copy number files (json) that can be exported from mesoscope.
- Report of the current total copy number.

Ingredient List and Fiber Ingredient List Panel :

- List of ingredients to distribute : ingredient id, compartment id and count can be specified.
- For fiber the total length, angle constraints, unit length and repetition in one unit length can be specified.

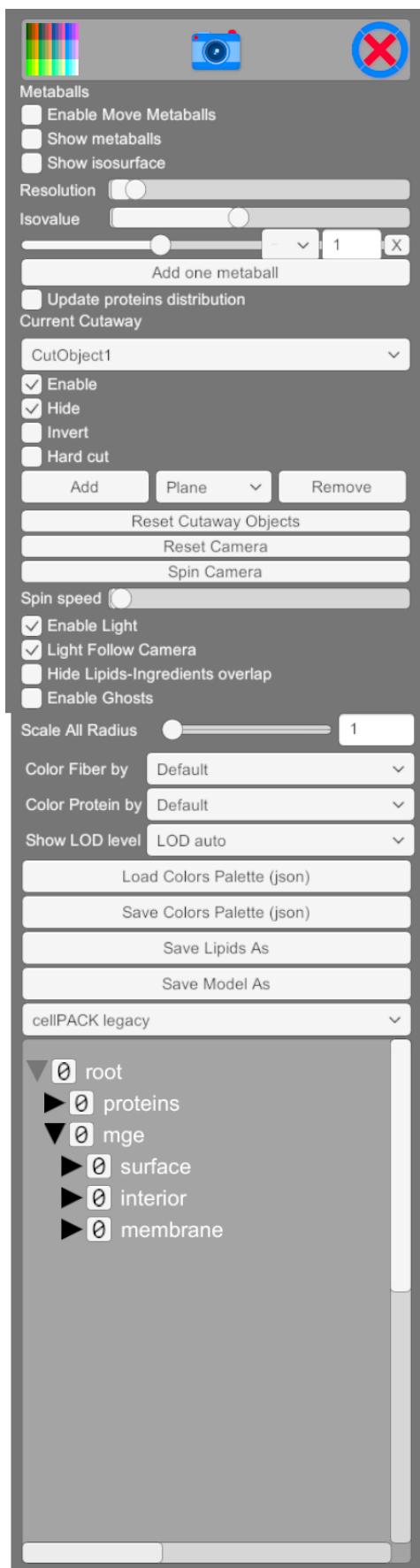
Lattices Model and TimeStamp :

- Pull down menu to switch between the automatic recipe and the curated recipe for Mycoplasma Genitalium
- Pull down menu to switch between the three frames extracted from the Whole cell computational model.
- Calculate the Persistence Length of the DNA

Overlap Relaxation :

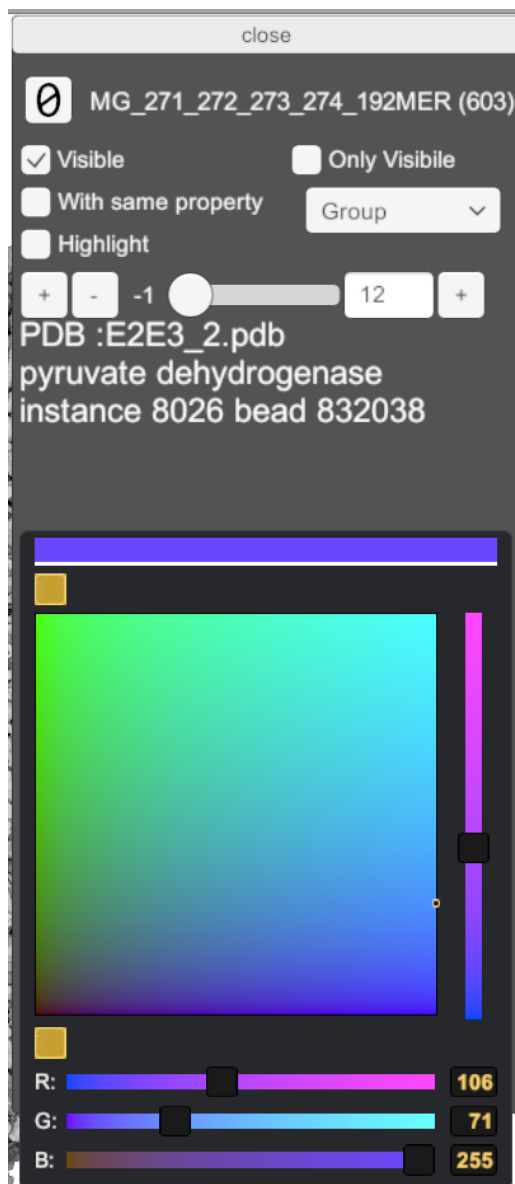
- Run on Step of relaxation
- Continuously run the relaxation
- Force reinitialisation
- Beads Level to use (flex use a unique radius for all particles, pick Lvl4 - Gpu can use larger and different beads radius, pick Lvl3).
- DNA persistence length constraints (spring between i,i+n beads)
- Show the beads lvl selected
- Show clashes (compute distance between beads of selected lvl)
- Relaxation mode : GPU / Flex / Flex Shared Memory
 - GPU: you can scale the displacement and torque force. Options consist in resolving compartment overlap, evaluating molecule-molecule overlap inside and at the surface, looking at fiber overlap and finally a special option to only evaluate the selection.
 - Flex : Toggle for drawing the flex particles and springs. Toggle for running the radius scaling loop (the unique particle radius increase/decrease in a loop). Maximum radius value to expand to. Label for the current radius. Slider for the Damping and the gravity forces. Final special button to fix the current selection during the initialisation. The fixed selection will act as a static collider.
 - Flex Shared memory : execute a standalone flex application which will share the molecules position/rotation in real time. Option are available directly in the standalone use interface.

Right Panel



- Change background color and transparency
- Take a screenshot
- Quit
- Enable Move Metaballs : Metabale can be manipulated with an handle (ctrl+click)
- Show the Metaballs
- Show the resulting isosurface from the volume dual contouring method.
- Resolution of the dual contour volume
- Isovalue for the isosurface
- Radius scaling or the given metaball
- Add one metaball to the scene
- Toggle update proteins distribution when metaballs are moved/transform with the handle.
- Current Cutaway section
 - Select the current cutaway
 - Enable/Disable the cut object
 - Hide/Show the cut object
 - Invert the clipping
 - Hard cut (clip at the atomic level vs at the instance level)
 - Add a clipping object of the given type
 - Remove selected clipping object
 - Reset all the cutaway object
- Reset the camera transformation and rotation
- Spin the camera at the given spin
- Enable/Disable shadow
- Shadow light follow the camera
- Toggle the visibility of overlapping lipids (use the current beads lvi to evaluate if lipids overlap with proteins)
 - Enable ghosting (show contour of hidden/clipped macromolecules)
 - Scale the all rendered sphere radius by
 - Switch the fiber color mode
 - Switch the protein color mode
 - Show a given Level of Detail, force the rendering of that LOD
 - Load/Save color palette (json)
 - Save the current lipids bilayer (without holes and with lipids-lipids overlap)
 - Save the current models as (cellpack, bin, pdb or cif)
 - Hierarchical Tree user interface to control visiilibty for a given tripping object with a three state toggle (-1 force hidden, 0 clipped, 1 force not clipped)

Ctrl+click will select a molecule or a fiber and toggle on the ingredient panel.



Three state toggle for controlling visibility with the selected clipping object followed by name of the selected ingredient.

Toggle for visibility (force hide or force show the ingredient).

Display every object share the same property (pull down menu of properties)

Highlight the selected molecule.

Control the current copy number.

Label reporting the PDB used, and the description of the ingredient.

Followed by the instance id and the bead id the user clicked on.

Color map to change the assigned ingredient color.