Visibility Equalizer Cutaway Visualization of Mesoscopic Biological Models

M. Le Muzic[1], P. Mindek[1], J. Sorger[1,2], L. Autin[3], D. Goodsell[3], I. Viola[1]

[1] TU Wien, Vienna, Austria

[2] VRVis Research Center, Vienna, Austria

[3] The Scripps Research Institute, La Jolla, California, USA

Overview

- Visibility **equalizer**

Visibility equalizer?

- This **equalizer**?

Equalizer?

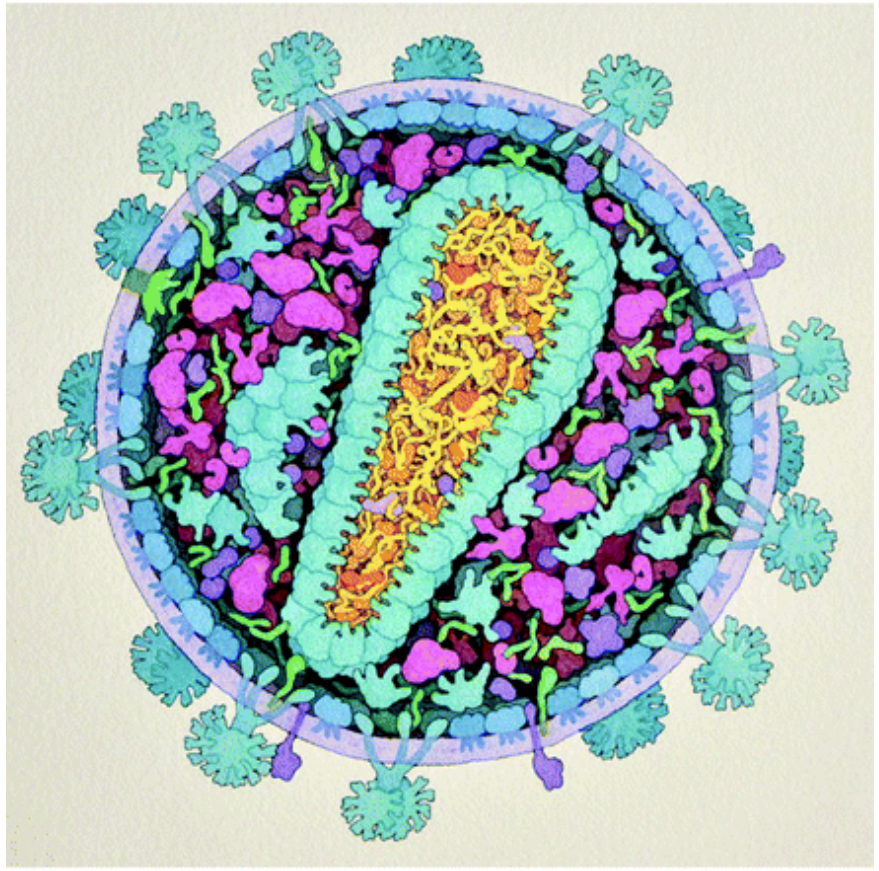
- No!!! This is **the equalizer** you should be thinking of!!!

Equalizer?

- Why?

Looks like we forgot something….

- Mesoscopic Biological Models!



+

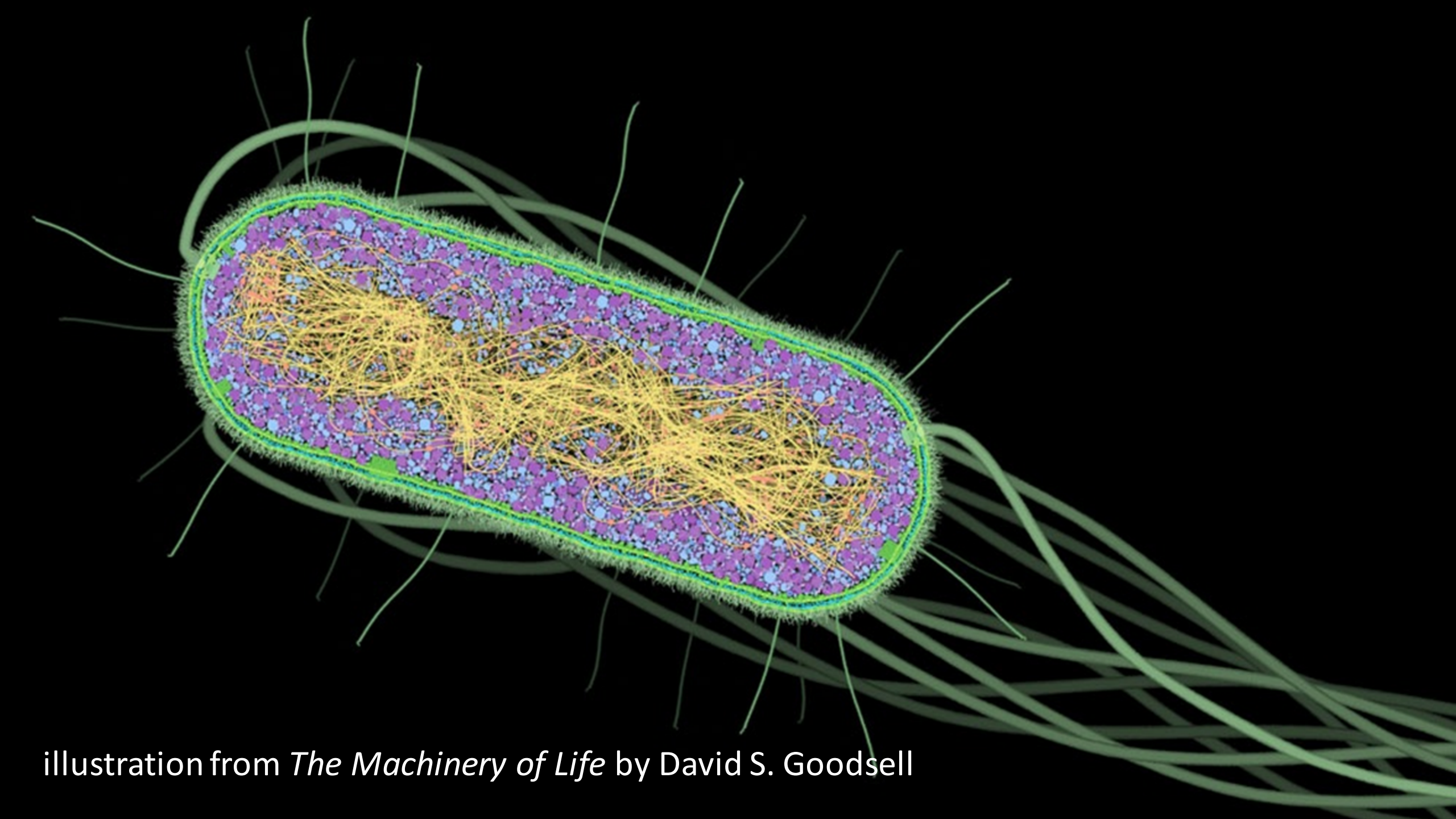
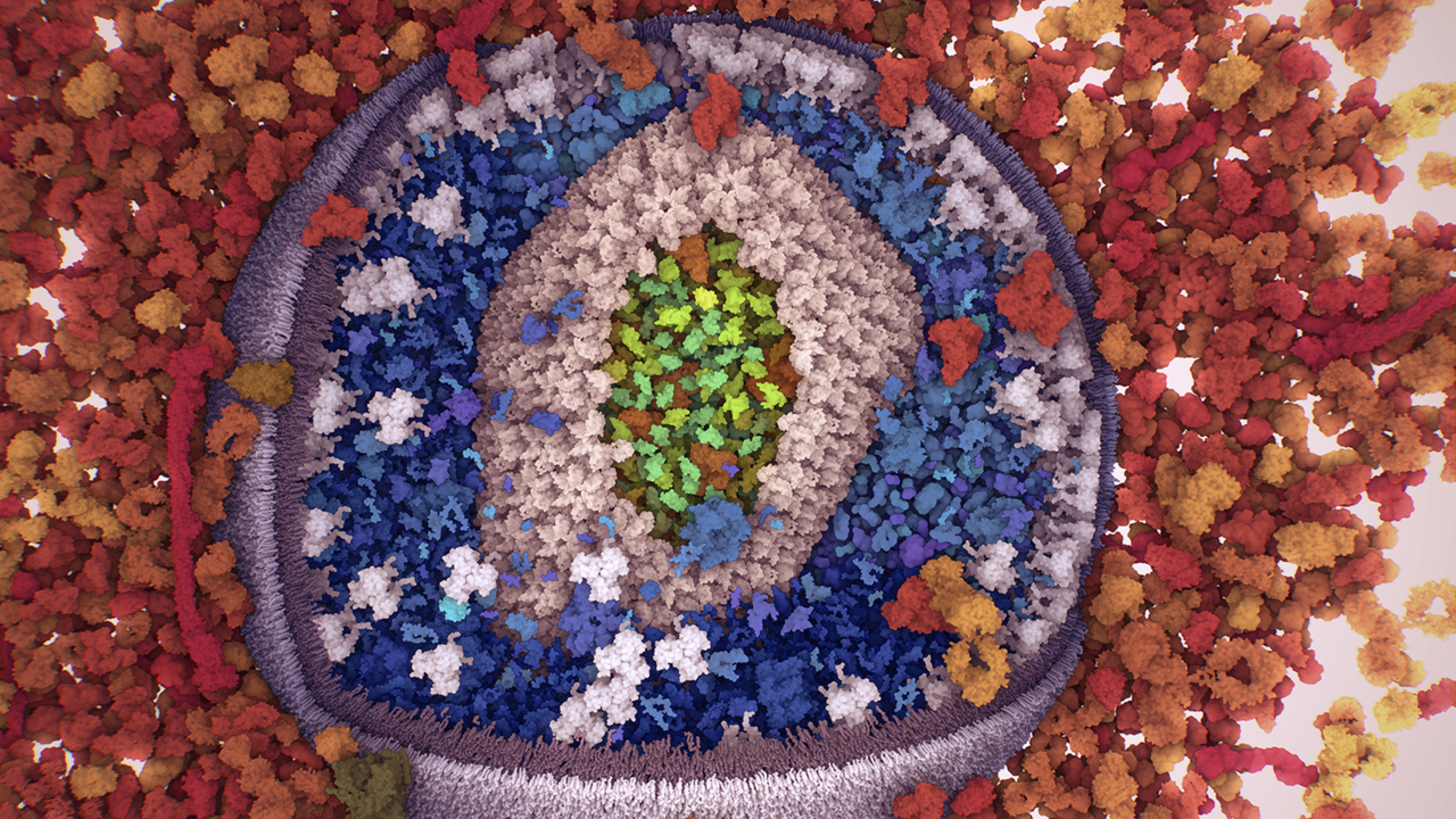
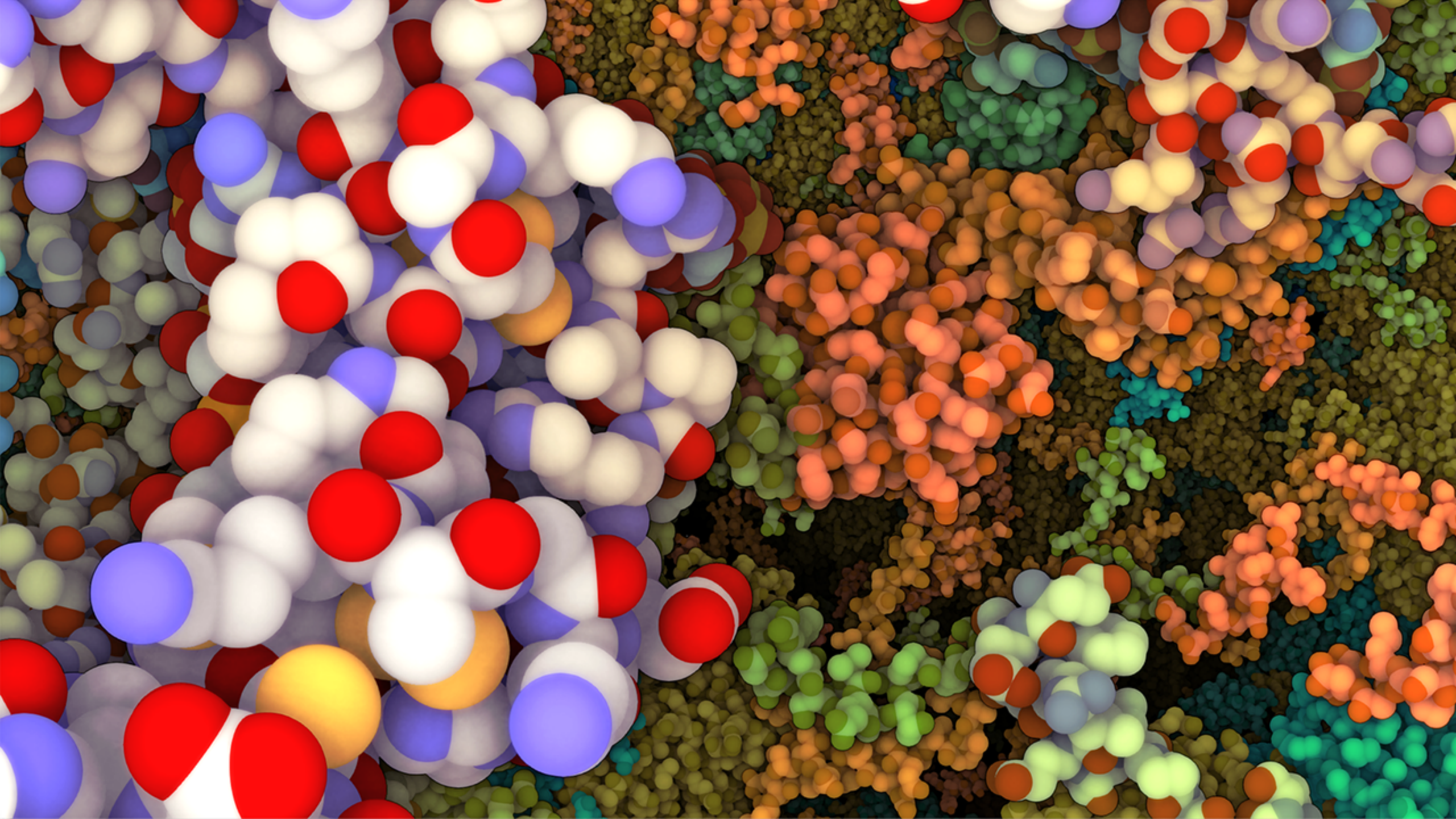


illustration from *The Machinery of Life* by David S. Goodsell

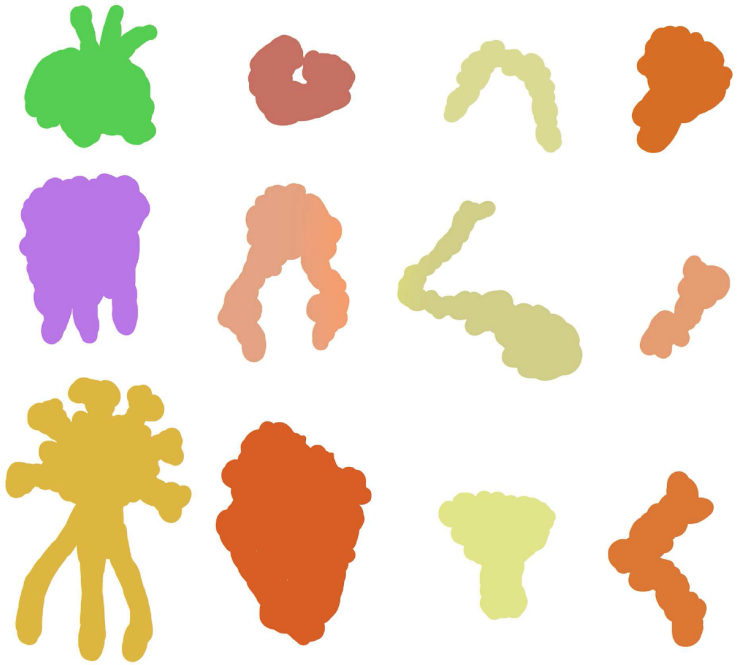
CellPack

- Procedural generation of 3D models that represent the structure of micro-organisms such as virus at atomic level. Given a set of parameters
  - molecular types
  - concentrations
  - spatial distribution



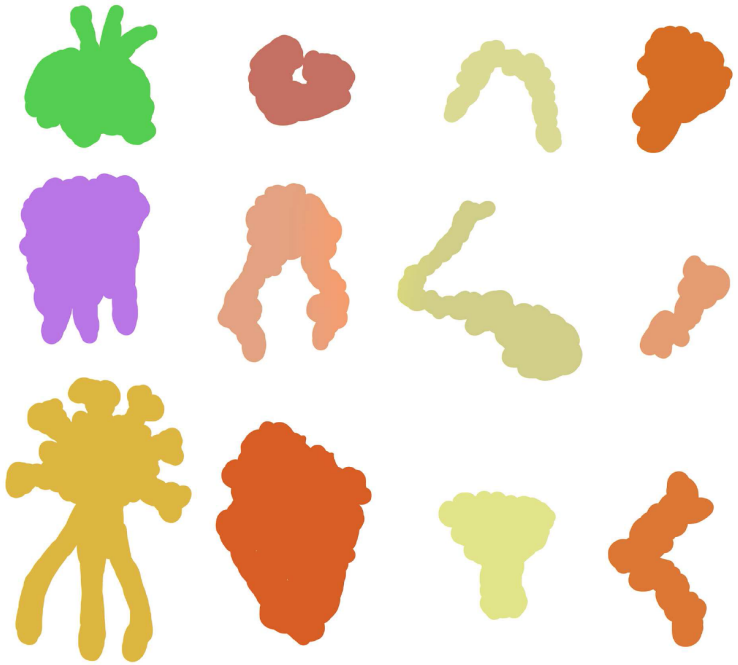


Mesoscopic Molecular Data

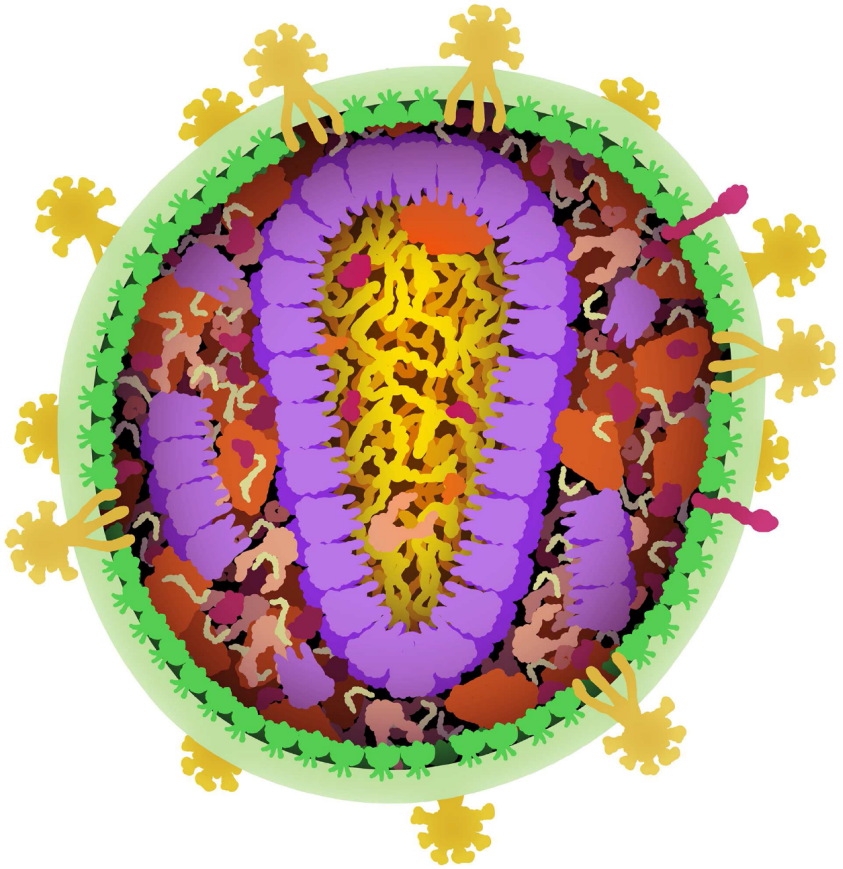


protein types

Mesoscopic Molecular Data



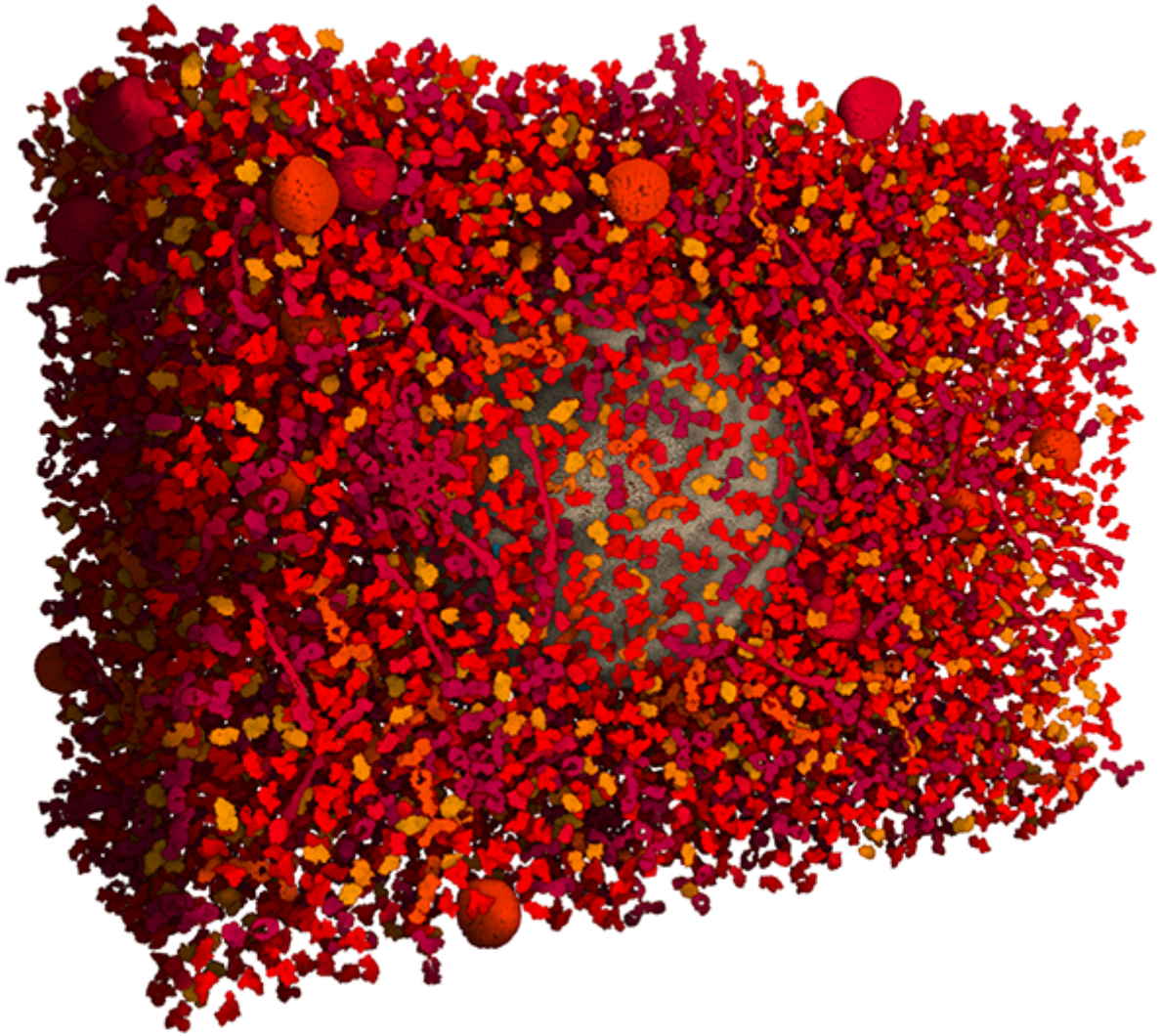
<



protein types

protein instances

Visibility within Dense Data



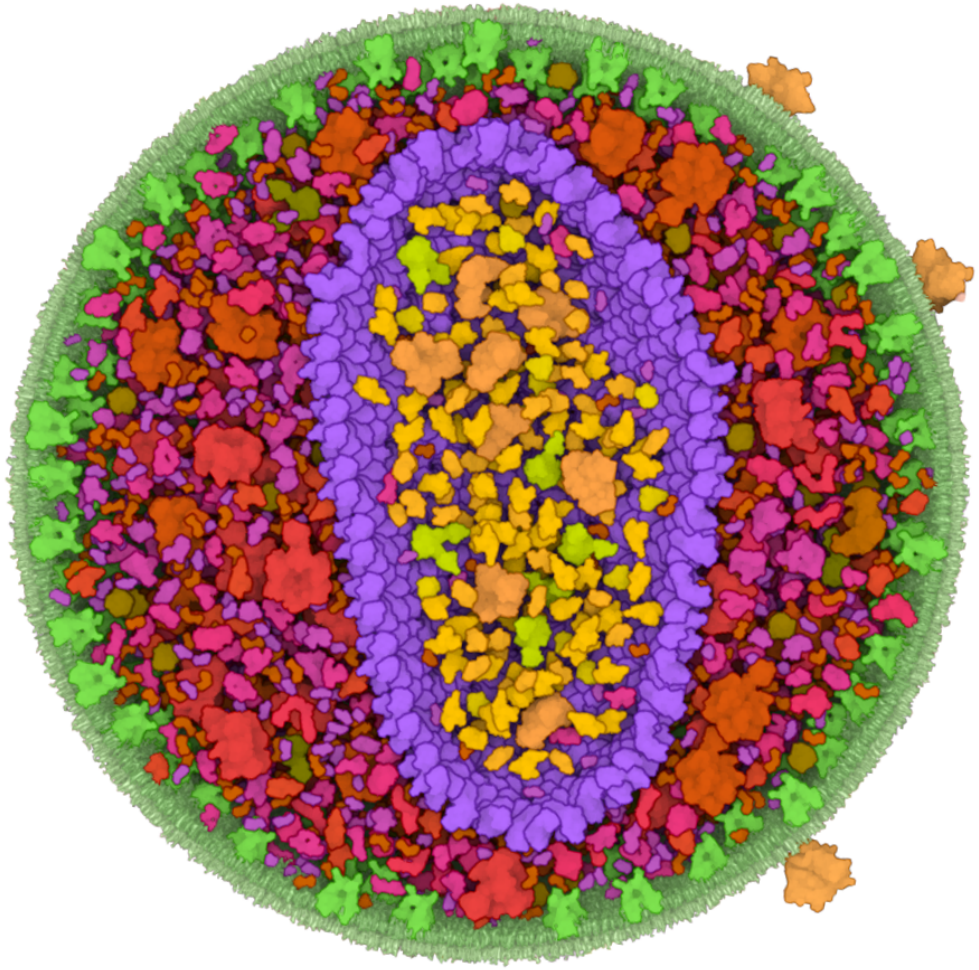
Cutaway Views

Cutaway Views

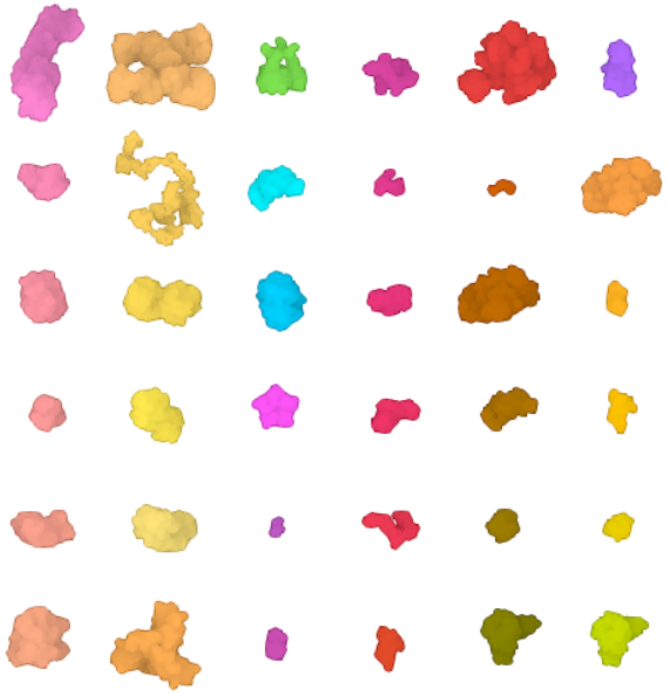
Illustration by David S. Goodsell

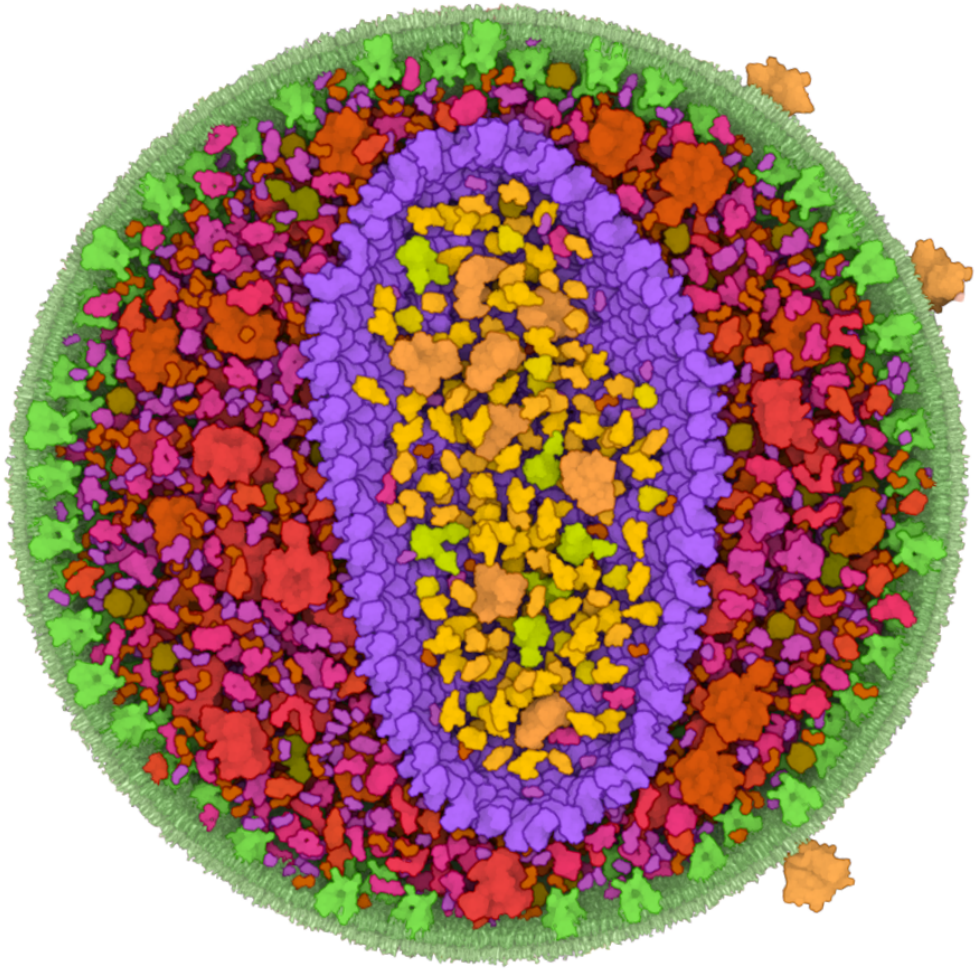
Illustration by David S. Goodsell

Which of the protein types are visible?



Which of the protein types are visible?

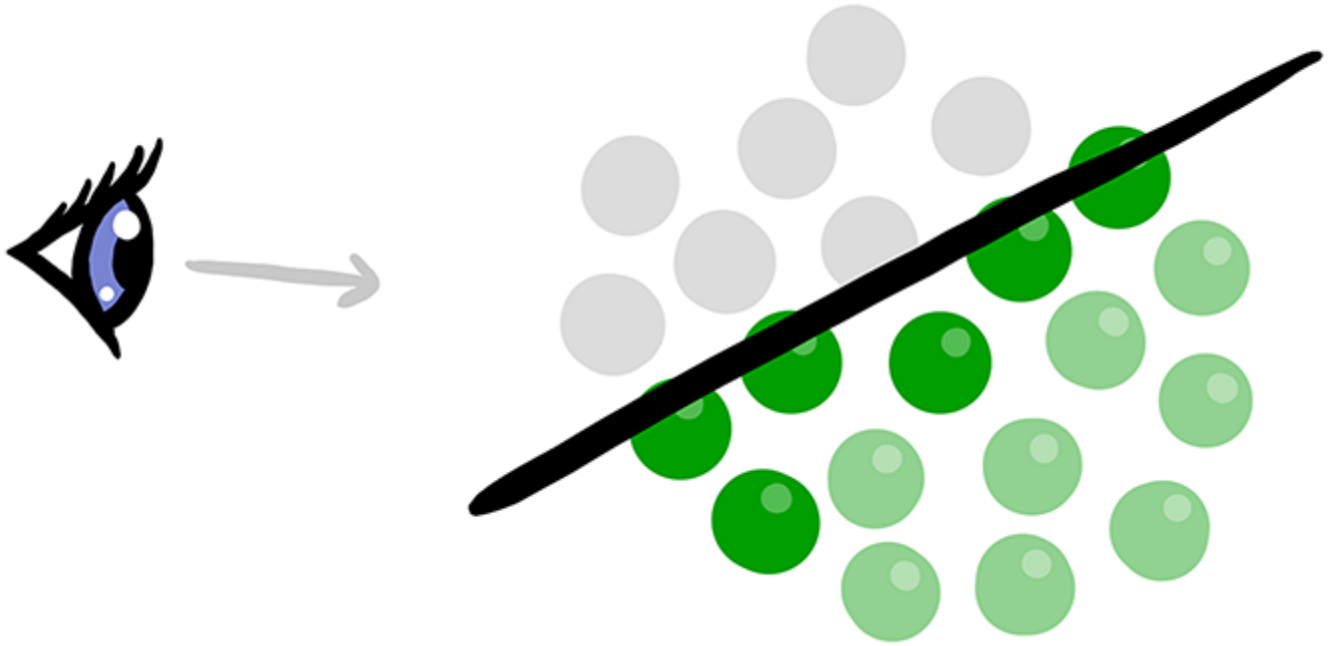




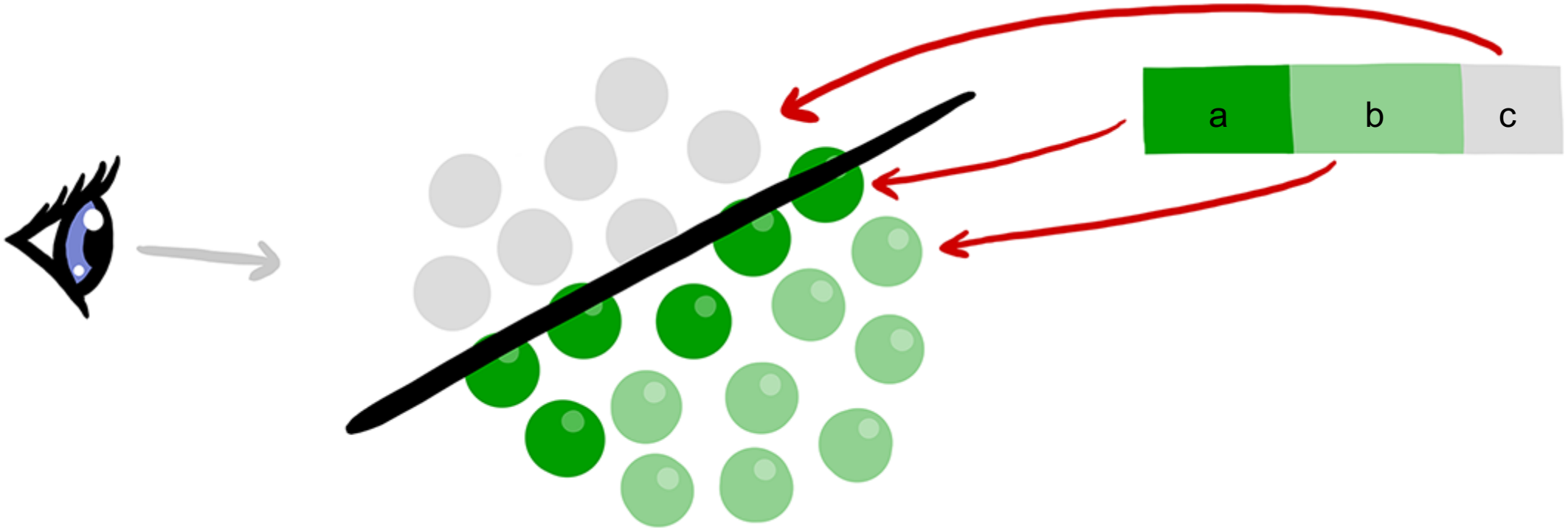
Contributions

- Method to quantify overall visibility
- Method to manage individual instances visibility
  - Visibility equalizer

Protein Visibility



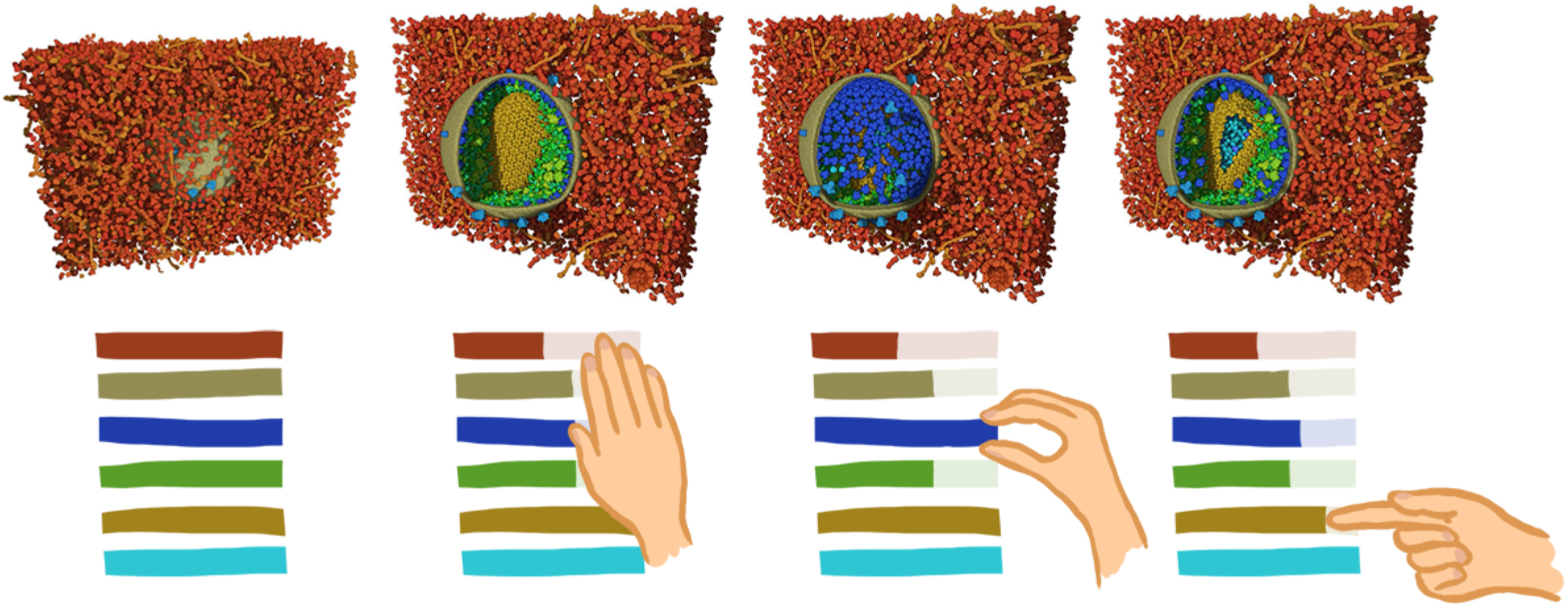
Protein Visibility



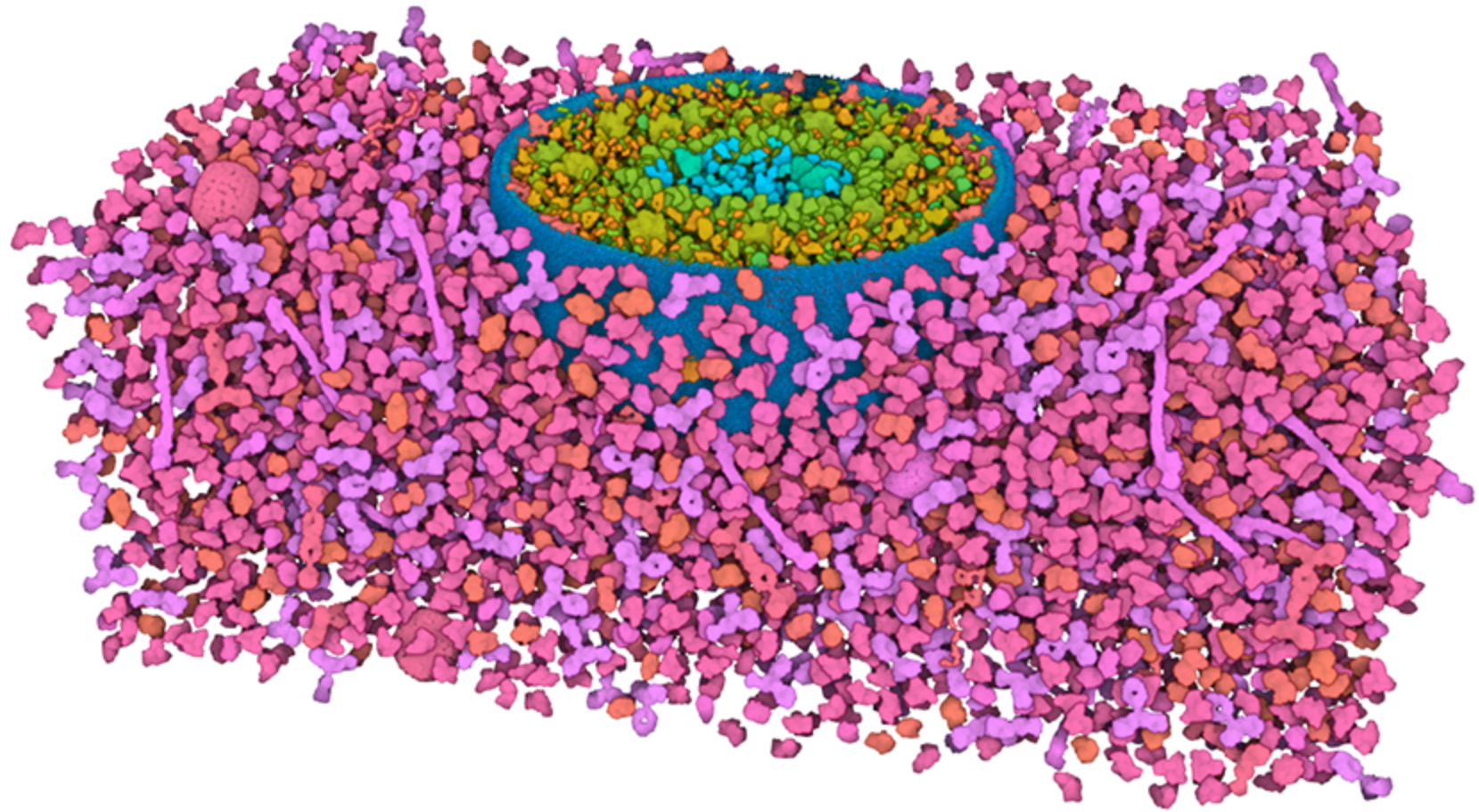
a - the ratio of visible instances to the total number of instances
b - the ratio of occluded instances to the total number of instances
c - the ratio of discarded instances to the total number of instances

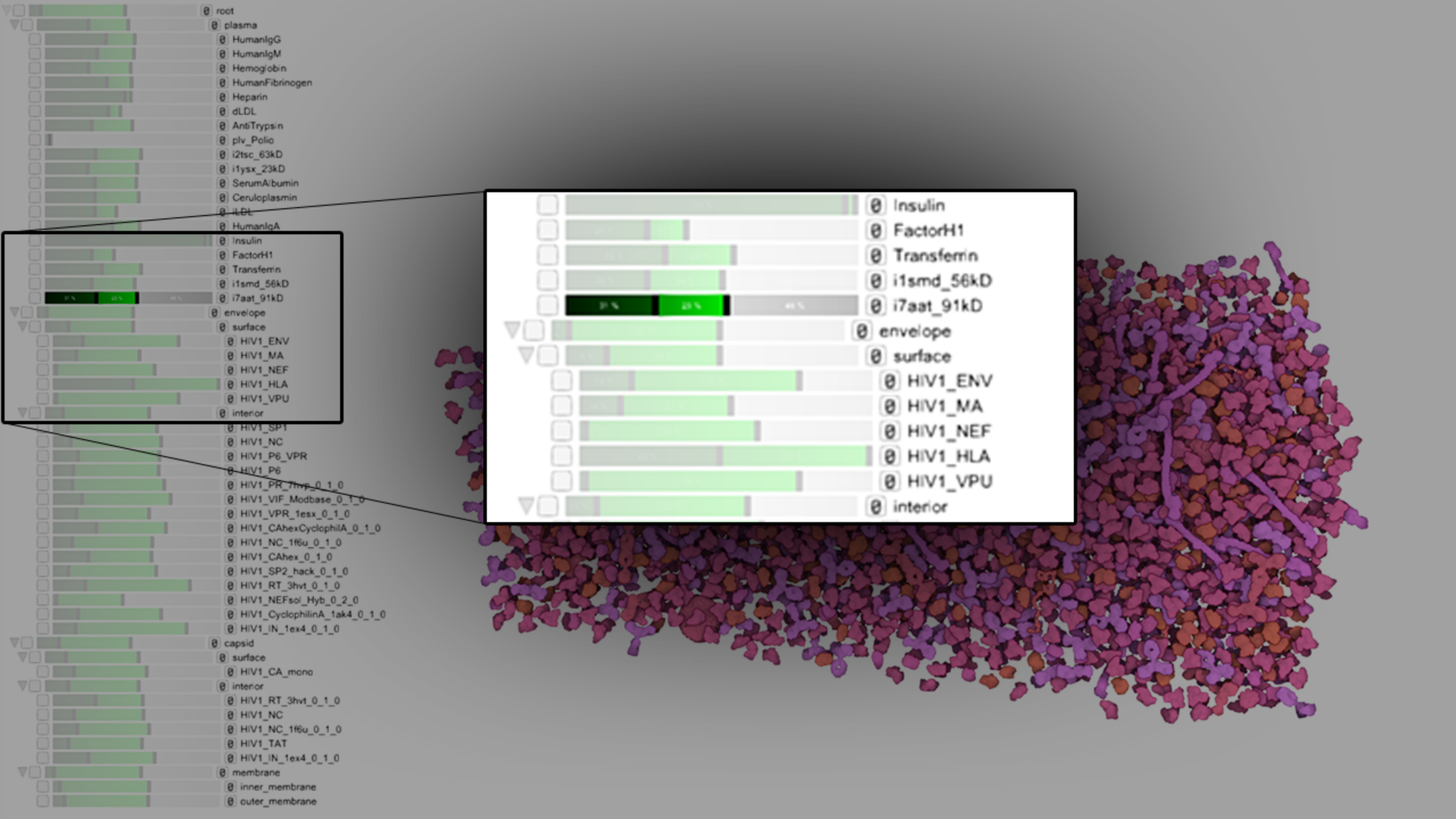
Equalizing Visibility

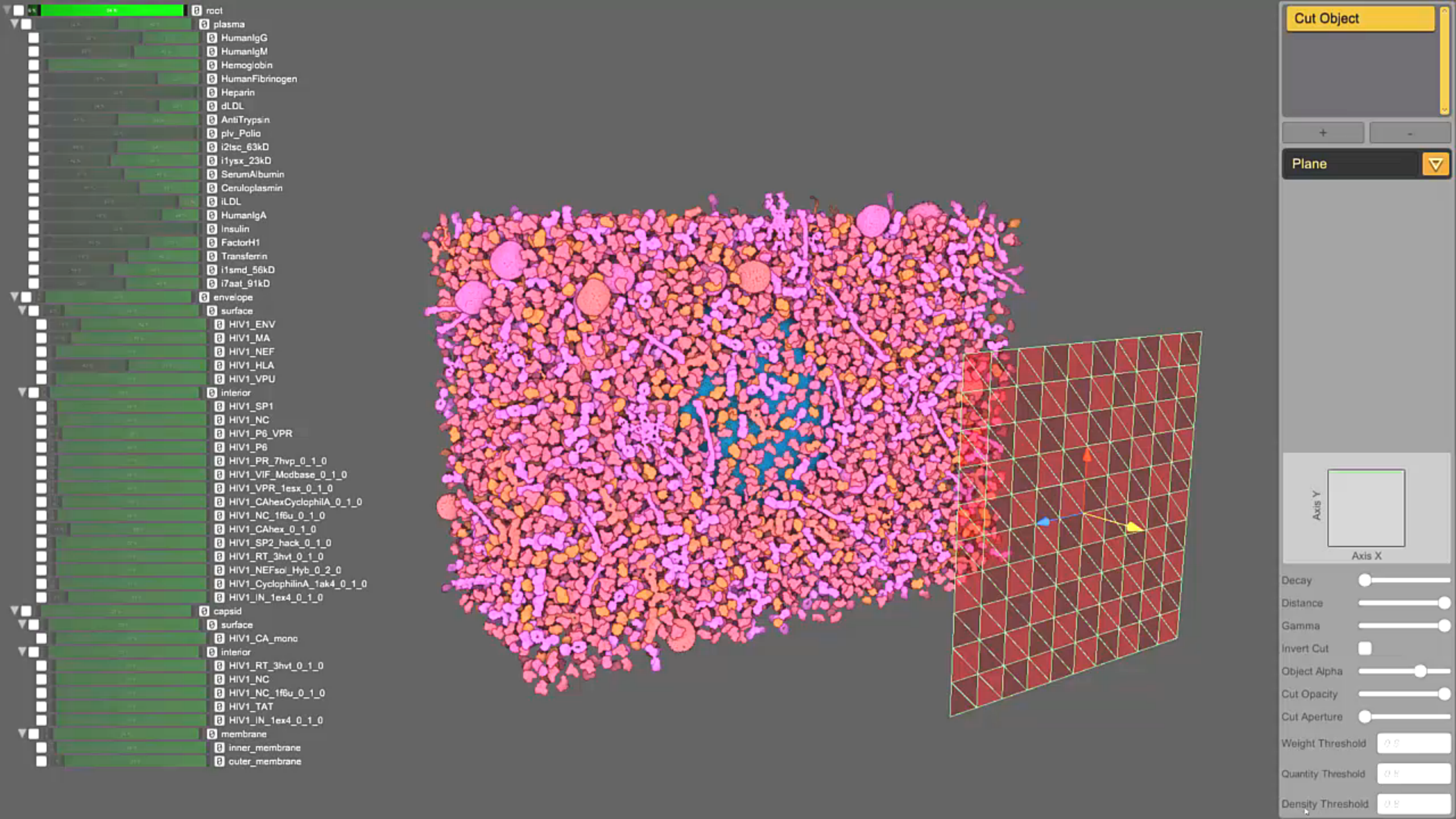
- Stacked bars used to **visualize** and to **interact**



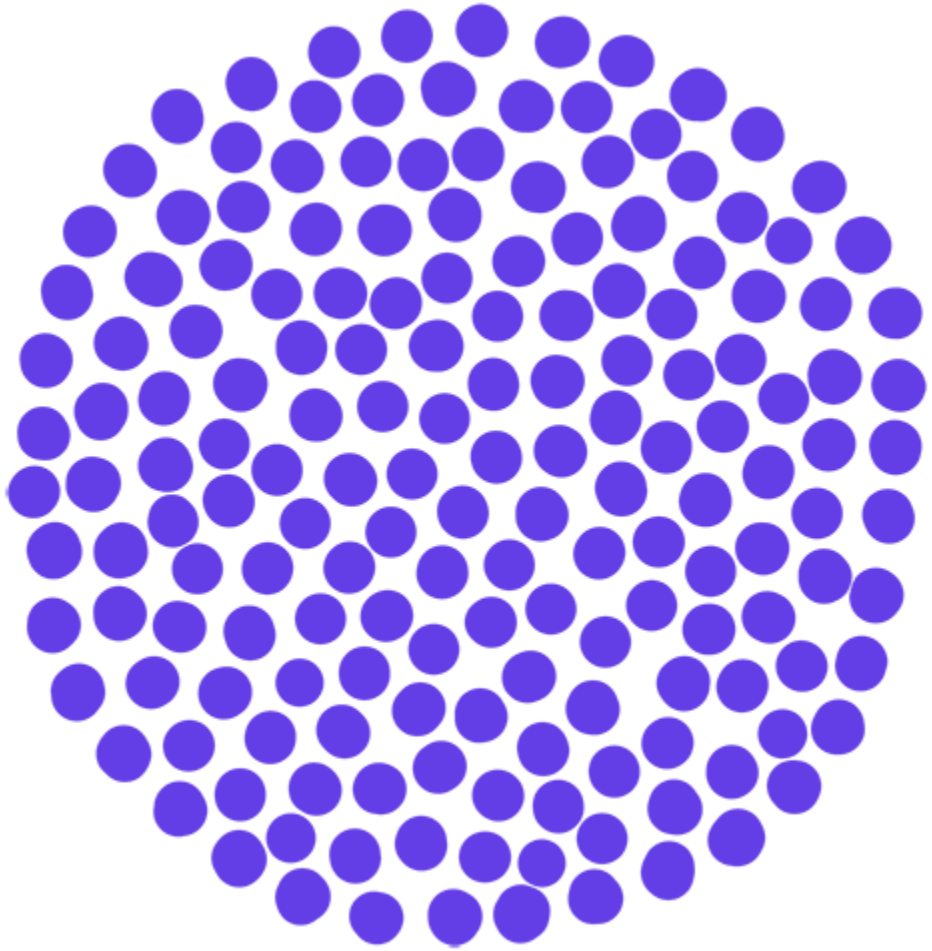
- root
  - plasma
    - HumanIgG
    - HumanIgM
    - Hemoglobin
    - HumanFibrinogen
    - Heparin
    - dLDL
    - AntiTrypsin
    - plv_Polio
    - i2tsc_63kD
    - i1ysx_23kD
    - SerumAlbumin
    - Ceruloplasmin
    - iLDL
    - HumanIgA
    - Insulin
    - FactorH1
    - Transferrin
    - i1smd_56kD
    - i7aat_91kD
  - envelope
    - surface
      - HIV1_ENV
      - HIV1_MA
      - HIV1_NEF
      - HIV1_HLA
      - HIV1_VPU
    - interior
      - HIV1_SP1
      - HIV1_NC
      - HIV1_P6_VPR
      - HIV1_P6
      - HIV1_PR_7hvp_0_1_0
      - HIV1_VIF_Modbase_0_1_0
      - HIV1_VPR_1esx_0_1_0
      - HIV1_CAhexCyclophilA_0_1_0
      - HIV1_NC_1f6u_0_1_0
      - HIV1_CAhex_0_1_0
      - HIV1_SP2_hack_0_1_0
      - HIV1_RT_3hvt_0_1_0
      - HIV1_NEFsol_Hyb_0_2_0
      - HIV1_CyclophilinA_1ak4_0_1_0
      - HIV1_IN_1ex4_0_1_0
  - capsid
    - surface
      - HIV1_CA_mono
    - interior
      - HIV1_RT_3hvt_0_1_0
      - HIV1_NC
      - HIV1_NC_1f6u_0_1_0
      - HIV1_TAT
      - HIV1_IN_1ex4_0_1_0
  - membrane
    - inner_membrane
    - outer_membrane



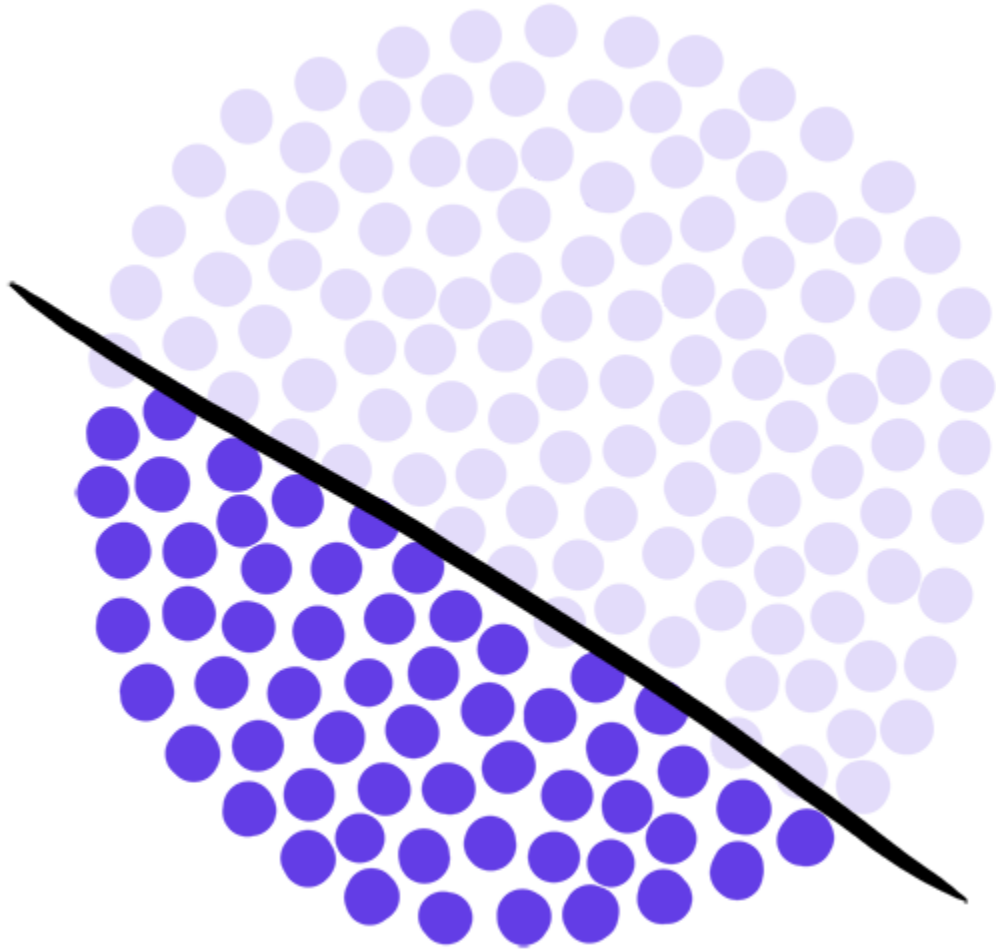

root
plasma
HumanIgG
HumanIgM
Hemoglobin
HumanFibrinogen
Heparin
dLDL
AntiTrypsin
plv_Polio
i2tsc_63kD
i1ysx_23kD
SerumAlbumin
Ceruloplasmin
iLDL
HumanIgA
Insulin
FactorH1
Transferrin
i1smd_56kD
i7aat_91kD
envelope
surface
HIV1_ENV
HIV1_MA
HIV1_NEF
HIV1_HLA
HIV1_VPU
interior
HIV1_SP1
HIV1_NC
HIV1_P6_VPR
HIV1_P6
HIV1_PR_7hvp_0_1_0
HIV1_VIF_Modbase_0_1_0
HIV1_VPR_1esx_0_1_0
HIV1_CAhexCyclophilA_0_1_0
HIV1_NC_1f6u_0_1_0
HIV1_CAhex_0_1_0
HIV1_SP2_hack_0_1_0
HIV1_RT_3hvt_0_1_0
HIV1_NEFsol_Hyb_0_2_0
HIV1_CyclophilinA_1ak4_0_1_0
HIV1_IN_1ex4_0_1_0
capsid
surface
HIV1_CA_mono
interior
HIV1_RT_3hvt_0_1_0
HIV1_NC
HIV1_NC_1f6u_0_1_0
HIV1_TAT
HIV1_IN_1ex4_0_1_0
membrane
inner_membrane
outer_membrane
Insulin
FactorH1
Transferrin
i1smd_56kD
i7aat_91kD
envelope
surface
HIV1_ENV
HIV1_MA
HIV1_NEF
HIV1_HLA
HIV1_VPU
interior


root
plasma
HumanIgG
HumanIgM
Hemoglobin
HumanFibrinogen
Heparin
dLDL
AntiTrypsin
plv_Polio
i2tsc_63kD
i1ysx_23kD
SerumAlbumin
Ceruloplasmin
iLDL
HumanIgA
Insulin
FactorH1
Transferrin
i1smd_56kD
i7aat_91kD
envelope
surface
HIV1_ENV
HIV1_MA
HIV1_NEF
HIV1_HLA
HIV1_VPU
interior
HIV1_SP1
HIV1_NC
HIV1_P6_VPR
HIV1_P6
HIV1_PR_7hvp_0_1_0
HIV1_VIF_Modbase_0_1_0
HIV1_VPR_1esx_0_1_0
HIV1_CAhexCyclophilA_0_1_0
HIV1_NC_1f6u_0_1_0
HIV1_CAhex_0_1_0
HIV1_SP2_hack_0_1_0
HIV1_RT_3hvt_0_1_0
HIV1_NEFsoi_Hyb_0_2_0
HIV1_CyclophilinA_1ak4_0_1_0
HIV1_IN_1ex4_0_1_0
capsid
surface
HIV1_CA_mono
interior
HIV1_RT_3hvt_0_1_0
HIV1_NC
HIV1_NC_1f6u_0_1_0
HIV1_TAT
HIV1_IN_1ex4_0_1_0
membrane
inner_membrane
outer_membrane
Cut Object
+
-
Plane
Axis Y
Axis X
Decay
Distance
Gamma
Invert Cut
Object Alpha
Cut Opacity
Cut Aperture
Weight Threshold
Quantity Threshold
Density Threshold

Probabilistic Clipping

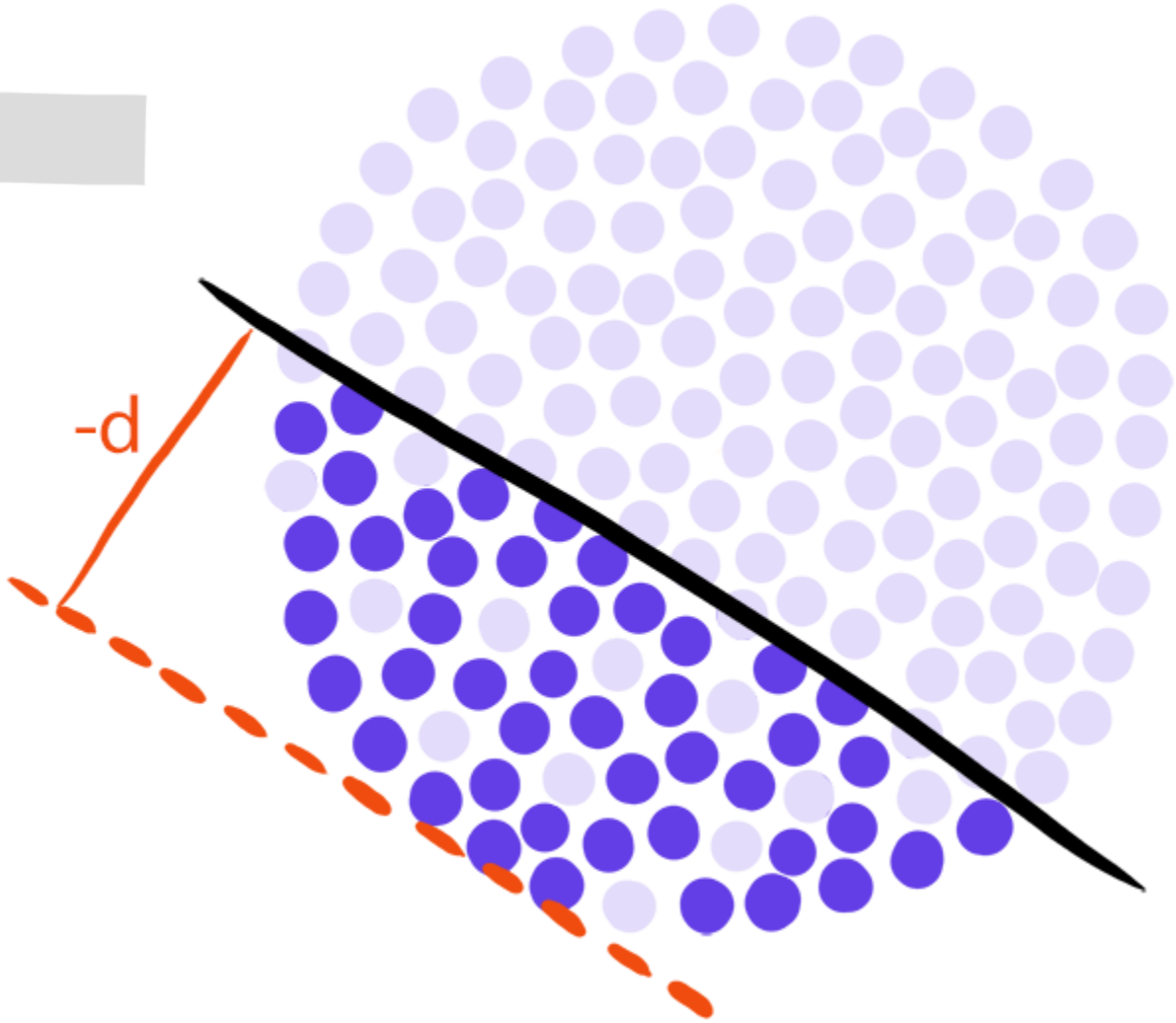


Probabilistic Clipping



Object-space clipping

Decreasing Clipping Probability



Object-space clipping

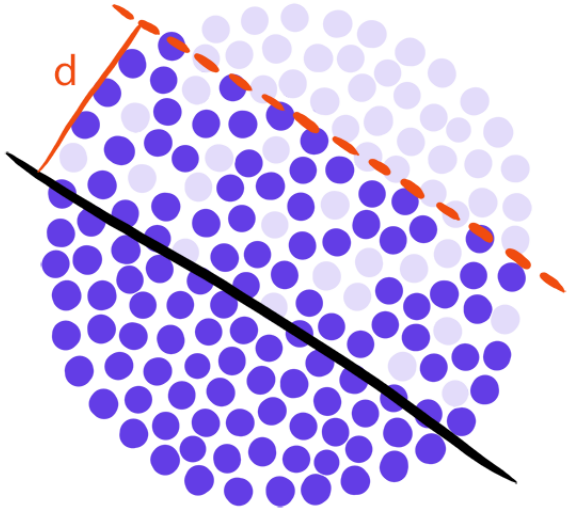
Clipping filtering

- The number of instances clipped can be fine tuned
  - Called *object-space clipping probability*
  - Controlled with the green-bar

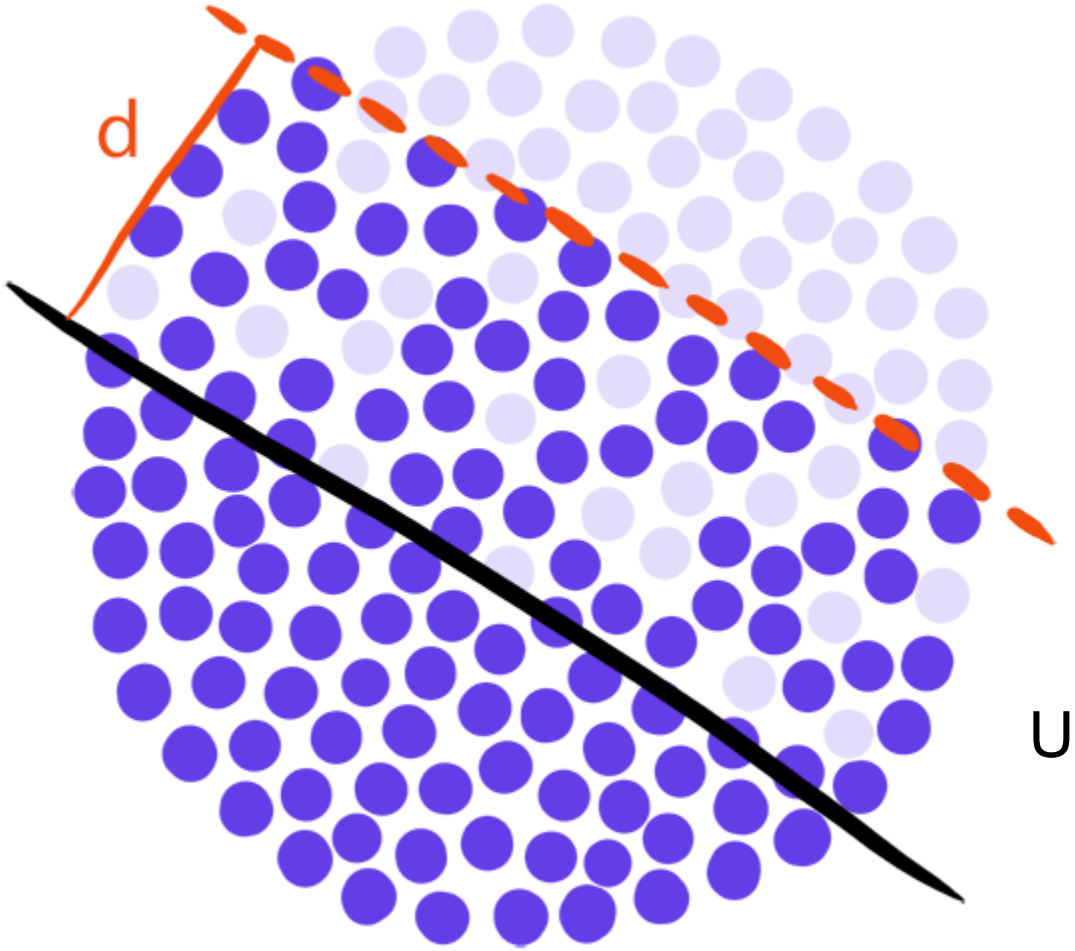
- Can filter with other properties
  - Molecular weight
  - Concentration

Object-space probabilistic clipping

- Upon start-up, each instance is given a clipping probability $p \in [0..1]$
  - The shader then acts:
    - If $p = 0$ → instance is clipped
    - If $p = 1$ → instance not clipped
    - If $p \in (0..1)$ → instance has a (1-p) probability of being clipped



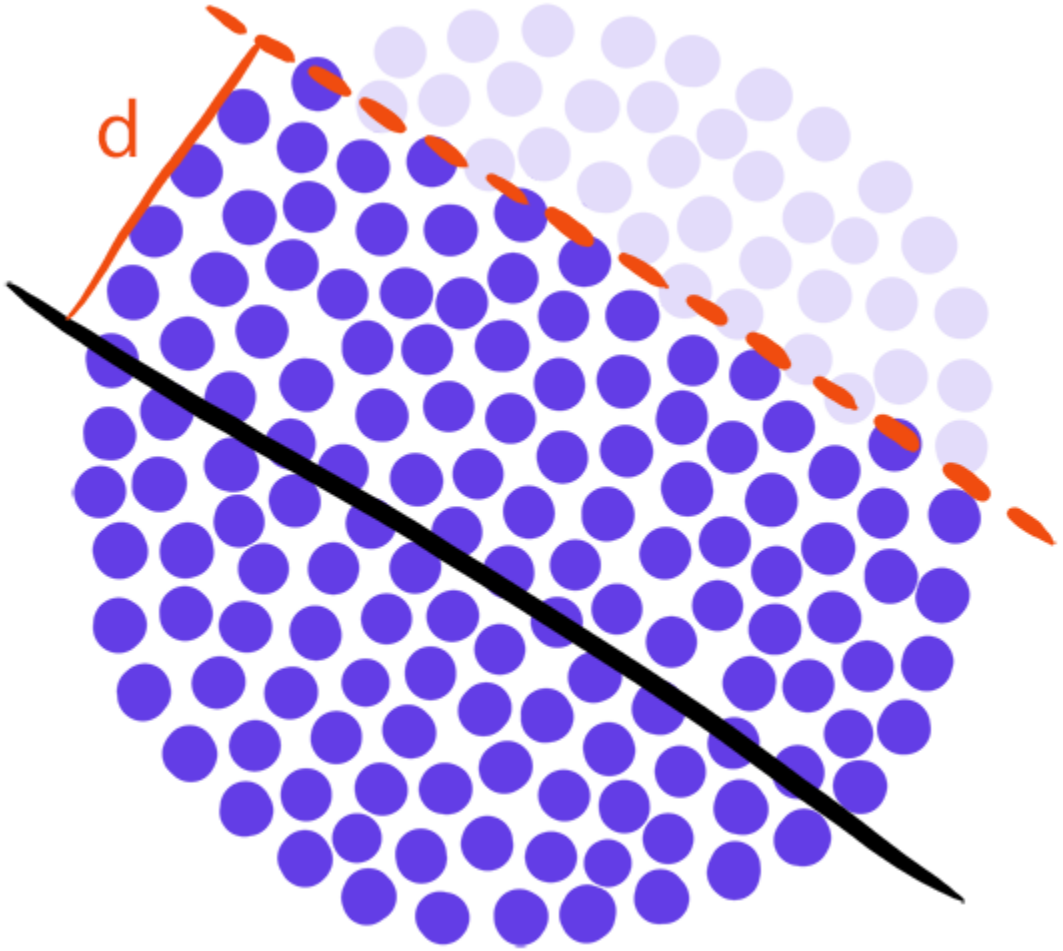
Decreasing Clipping Probability



Object-space clipping

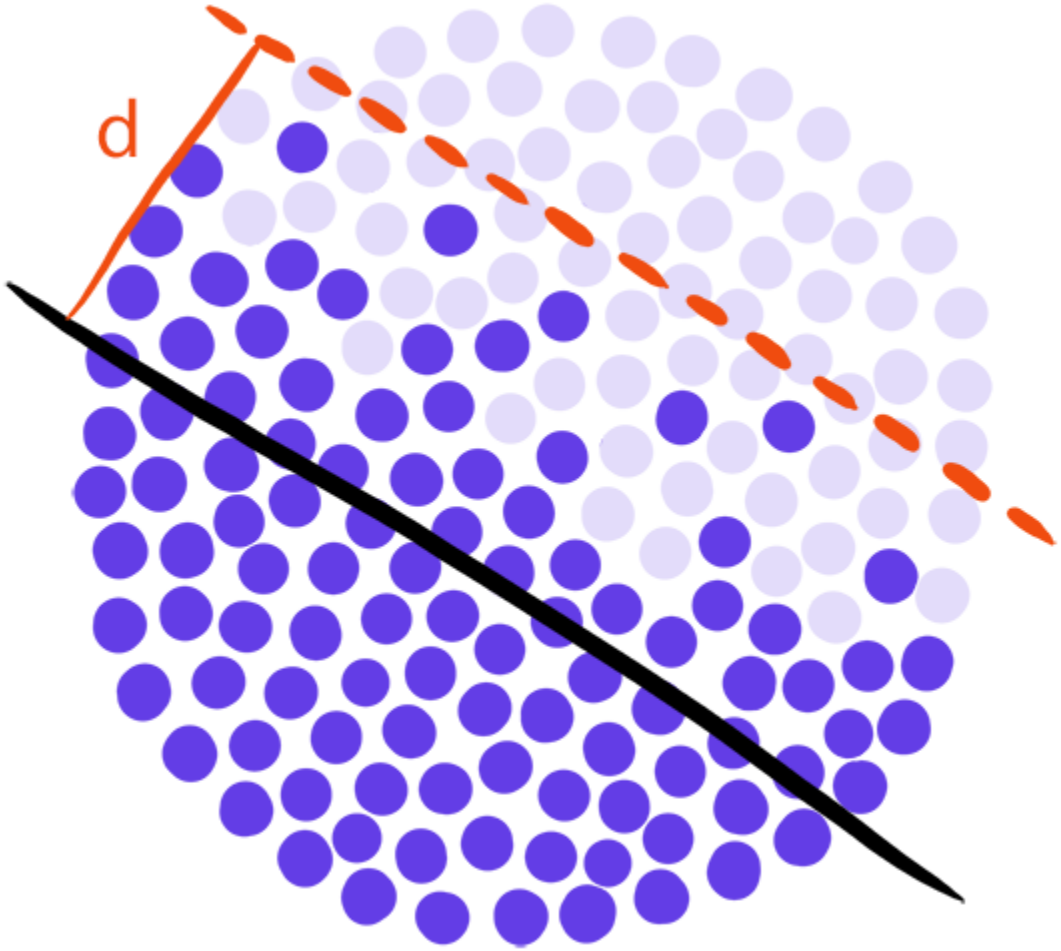
Uniform

Maximum Clipping Probability



Object-space clipping

Clipping Falloff



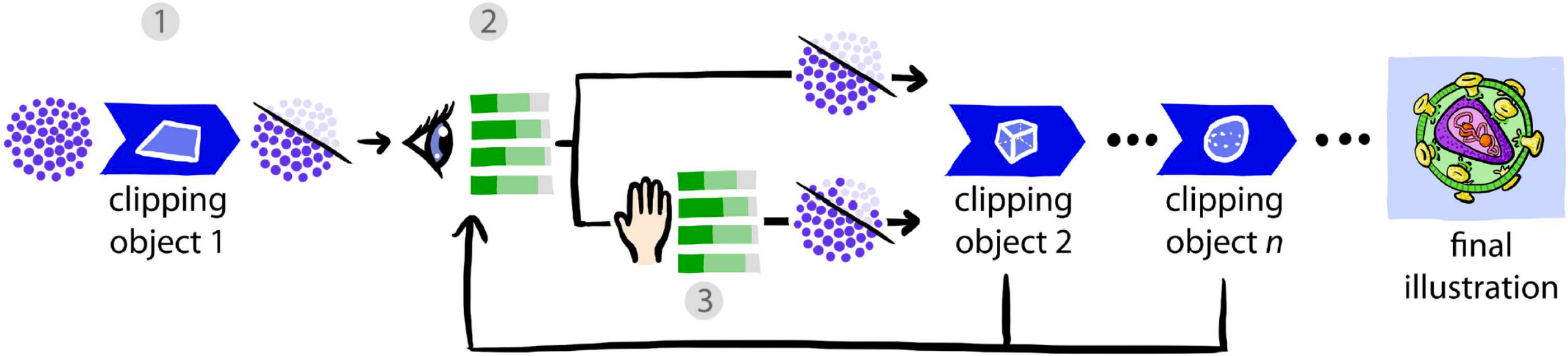
Object-space clipping

with a fall-off function

$$f(\vec{p}) = 1 - min(1, (d(\vec{p})/m)^c)$$

d(p): distance to the clipping surface from point p
m: maximum distance of object-space clipping

Workflow



- Loop

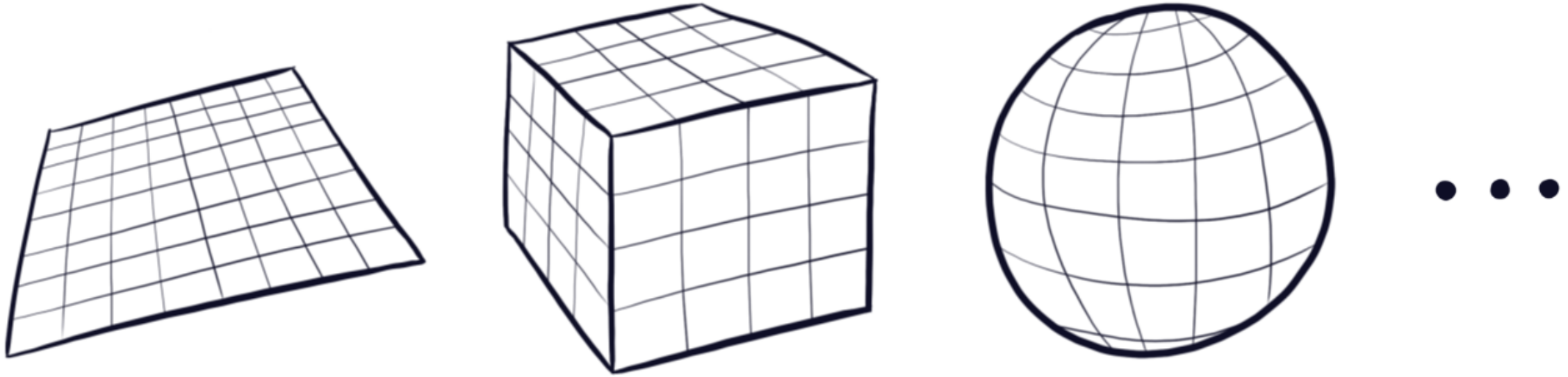
1. Add clipping object
2. Overall visibility calculation
3. Interact to obtain detailed visibility

Workflow

- Counting clipped instances
  - A dedicated compute shader queries the flags in the GPU memory
    - Stores the result in another structure
      - Per ingredient type
    - Use atomic operations
- Counting visible instances
  - Analogous to the previous one using a post-processing shader
- Resulting data is uploaded to CPU to update the equalizer values

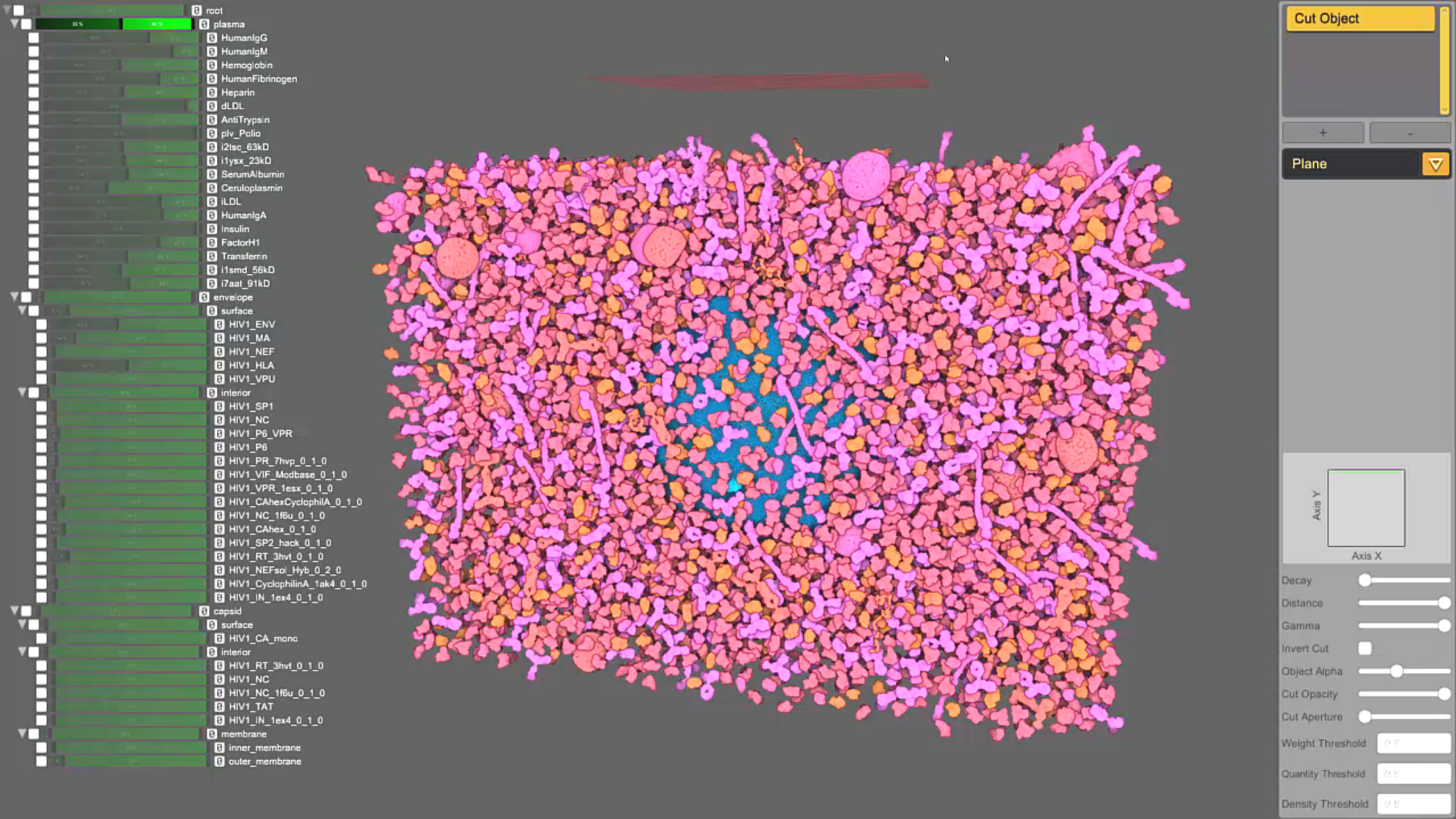
Workflow

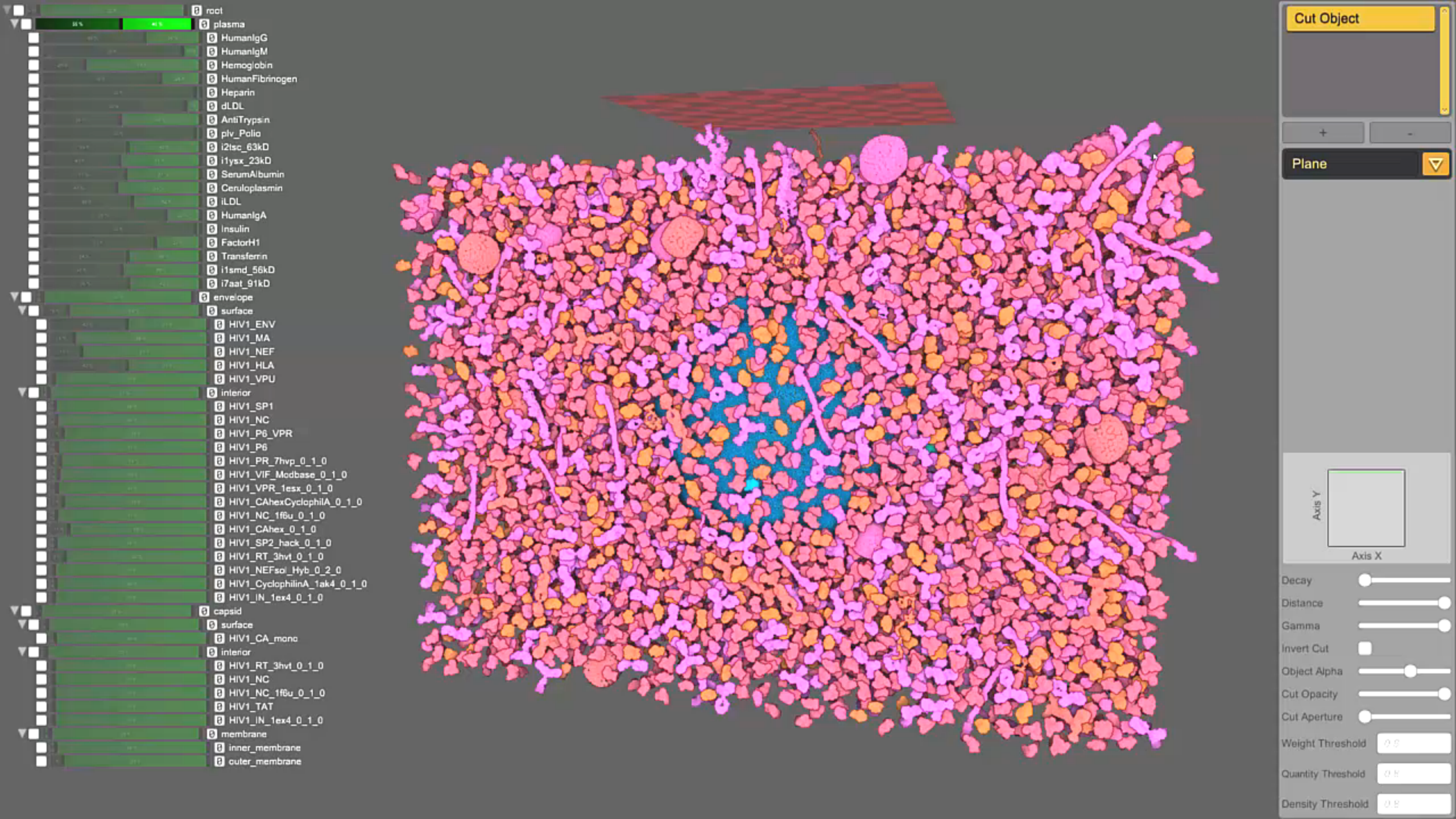
- Implicit clipping objects: Plane, cube, sphere, cylinder and cone



Workflow

- **Clipping** achieved with a 3D signed distance field per clipping object
  - Instances information (position, rotation, type, radius, etc.) are stored in large buffers on the GPU memory
  - Clipping (distance) computed in parallel in a compute shader program
    - one thread allocated per instance
  - When an object needs to be clipped, a dedicated flag in a GPU buffer is updated
    - The flag is then accessed during the rendering to discard the clipped instance


root
plasma
HumanIgG
HumanIgM
Hemoglobin
HumanFibrinogen
Heparin
dLDL
AntiTrypsin
plv_Polio
i2tsc_63kD
i1ysx_23kD
SerumAlbumin
Ceruloplasmin
iLDL
HumanIgA
Insulin
FactorH1
Transferrin
i1smd_56kD
i7aat_91kD
envelope
surface
HIV1_ENV
HIV1_MA
HIV1_NEF
HIV1_HLA
HIV1_VPU
interior
HIV1_SP1
HIV1_NC
HIV1_P6_VPR
HIV1_P6
HIV1_PR_7hvp_0_1_0
HIV1_VIF_Modbase_0_1_0
HIV1_VPR_1esx_0_1_0
HIV1_CAhexCyclophilA_0_1_0
HIV1_NC_1f6u_0_1_0
HIV1_CAhex_0_1_0
HIV1_SP2_hack_0_1_0
HIV1_RT_3hvt_0_1_0
HIV1_NEFsol_Hyb_0_2_0
HIV1_CyclophilinA_1ak4_0_1_0
HIV1_IN_1ex4_0_1_0
capsid
surface
HIV1_CA_mono
interior
HIV1_RT_3hvt_0_1_0
HIV1_NC
HIV1_NC_1f6u_0_1_0
HIV1_TAT
HIV1_IN_1ex4_0_1_0
membrane
inner_membrane
outer_membrane
Cut Object
+
-
Plane
Axis Y
Axis X
Decay
Distance
Gamma
Invert Cut
Object Alpha
Cut Opacity
Cut Aperture
Weight Threshold
Quantity Threshold
Density Threshold

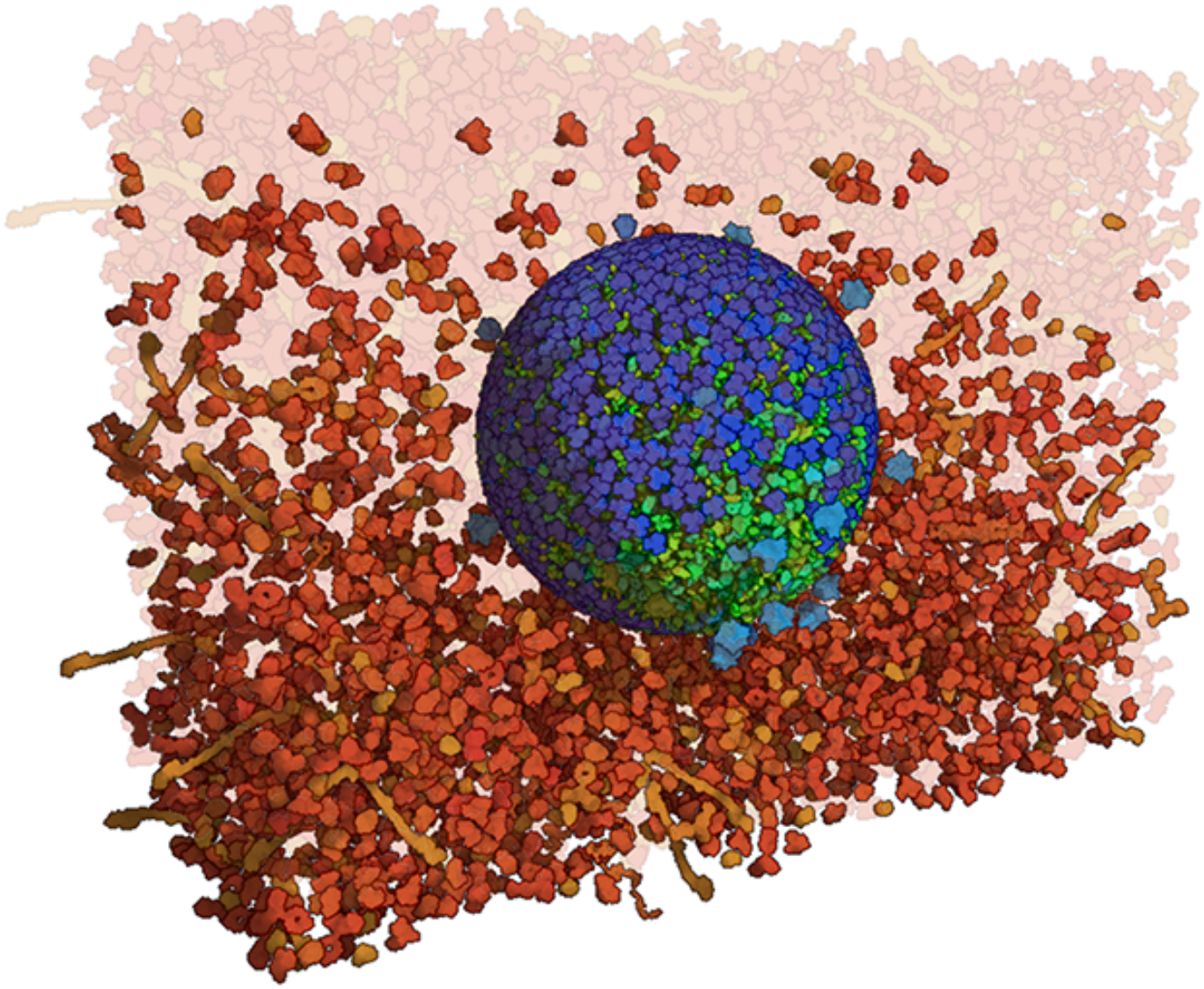

root
plasma
HumanIgG
HumanIgM
Hemoglobin
HumanFibrinogen
Heparin
dLDL
AntiTrypsin
plv_Polio
i2tsc_63kD
i1ysx_23kD
SerumAlbumin
Ceruloplasmin
iLDL
HumanIgA
Insulin
FactorH1
Transferrin
i1smd_56kD
i7aat_91kD
envelope
surface
HIV1_ENV
HIV1_MA
HIV1_NEF
HIV1_HLA
HIV1_VPU
interior
HIV1_SP1
HIV1_NC
HIV1_P6_VPR
HIV1_P6
HIV1_PR_7hvp_0_1_0
HIV1_VIF_Modbase_0_1_0
HIV1_VPR_1esx_0_1_0
HIV1_CAhexCyclophilA_0_1_0
HIV1_NC_1f6u_0_1_0
HIV1_CAhex_0_1_0
HIV1_SP2_hack_0_1_0
HIV1_RT_3hvt_0_1_0
HIV1_NEFsol_Hyb_0_2_0
HIV1_CyclophilinA_1ak4_0_1_0
HIV1_IN_1ex4_0_1_0
capsid
surface
HIV1_CA_mono
interior
HIV1_RT_3hvt_0_1_0
HIV1_NC
HIV1_NC_1f6u_0_1_0
HIV1_TAT
HIV1_IN_1ex4_0_1_0
membrane
inner_membrane
outer_membrane
Cut Object
+
-
Plane
Axis Y
Axis X
Decay
Distance
Gamma
Invert Cut
Object Alpha
Cut Opacity
Cut Aperture
Weight Threshold
Quantity Threshold
Density Threshold

Illustrative Techniques

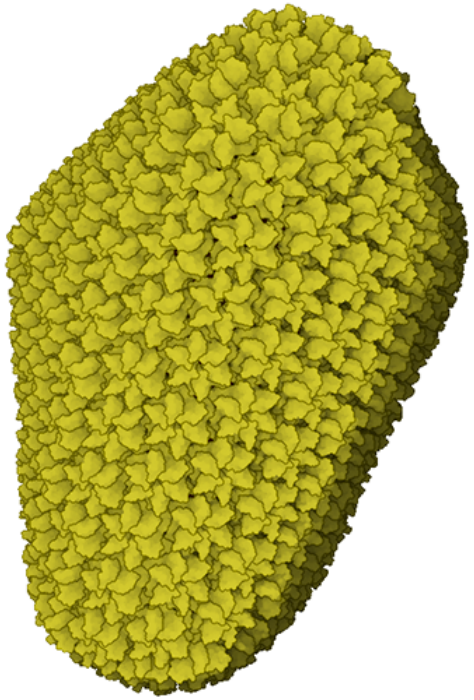
View-space clipping: Occluder removal

- Focused elements can be set as visible
  - **Occluders are removed** using occlusion queries
  1. Objects of interest are rendered offscreen with stencil and depth on
  2. Rest of the objects are rendered
     1. If they pass depth-stencil they are flagged to be skipped
  3. Render again

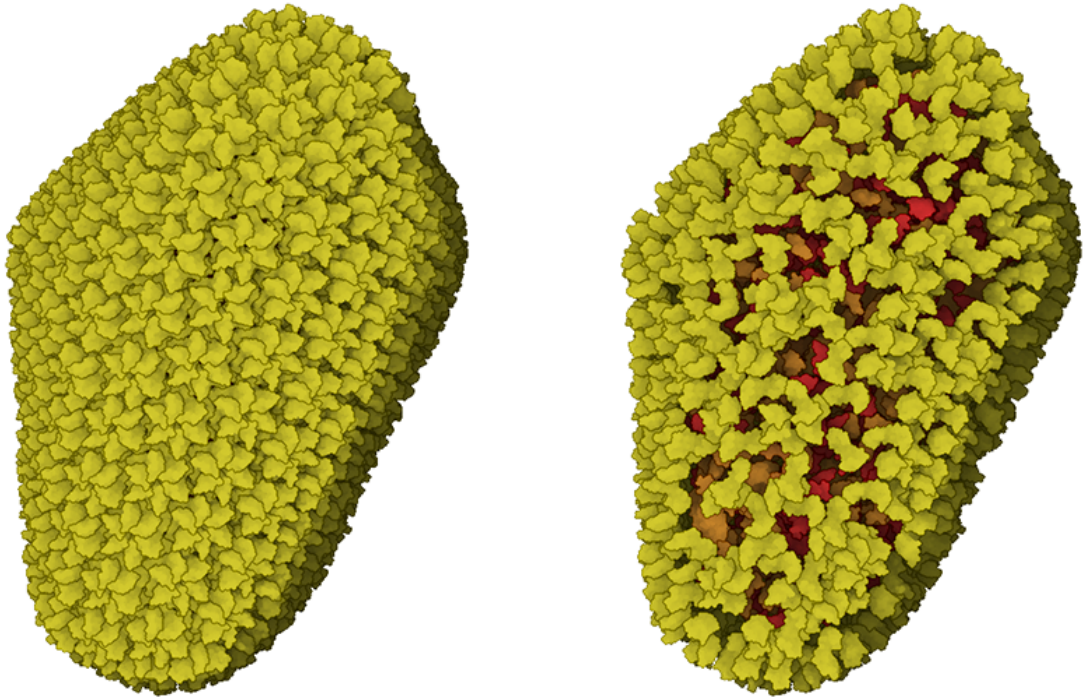
Ghosting



View-Space Clipping

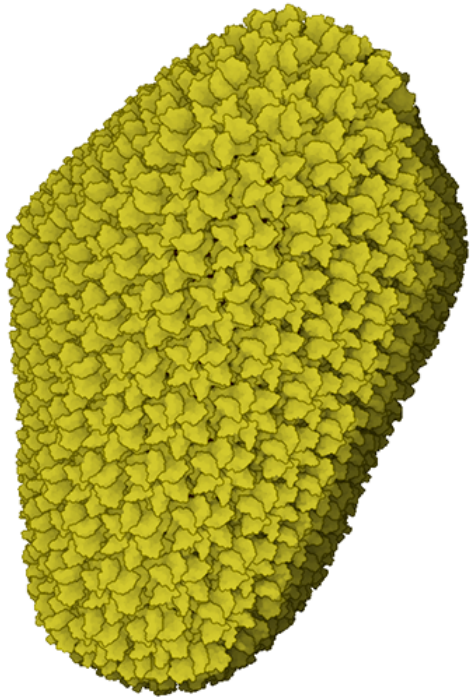


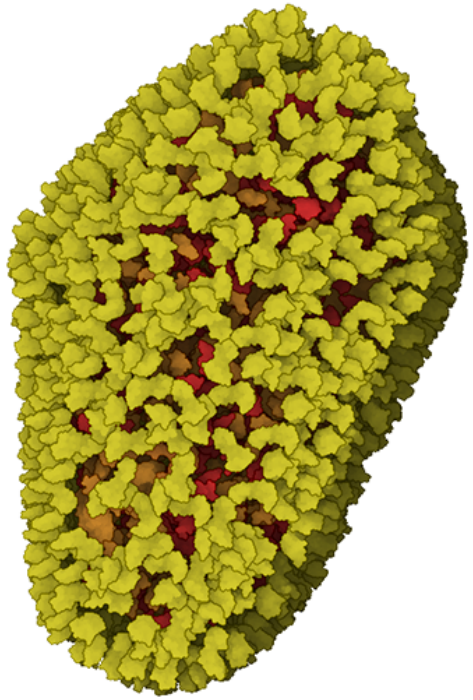
View-Space Clipping



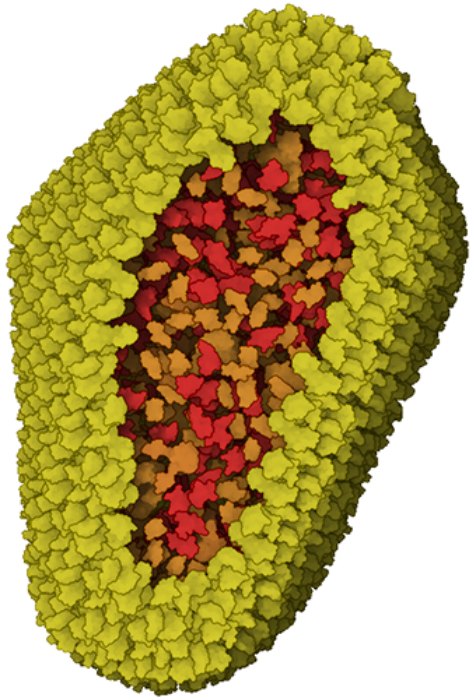
Uniform clipping

View-Space Clipping



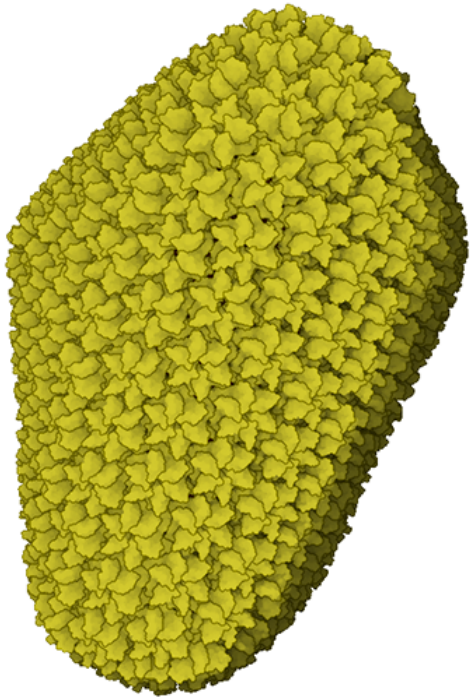


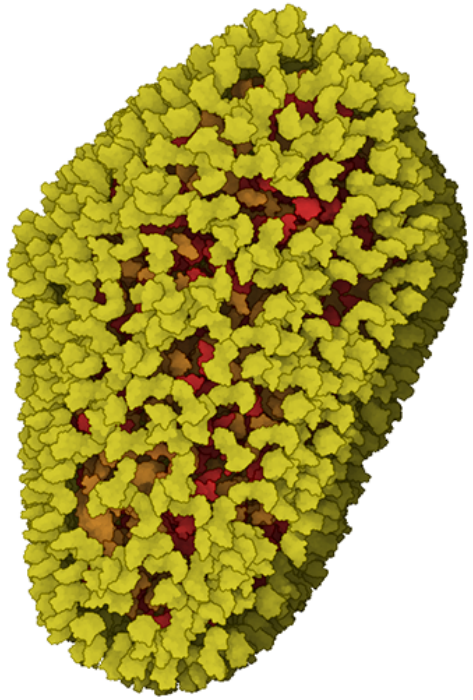
Uniform clipping



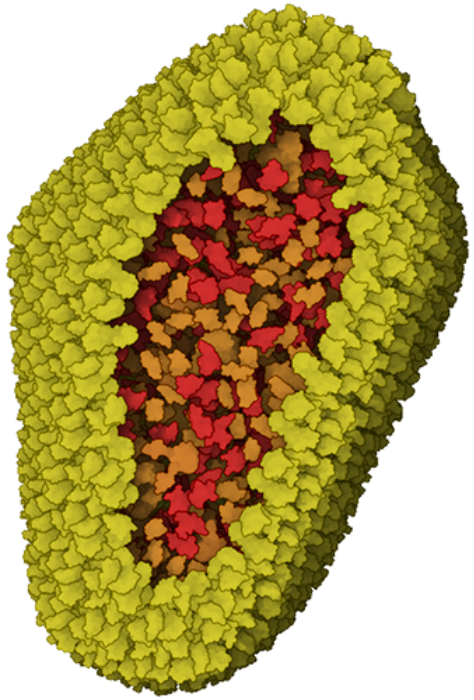
Aperture-based clipping

View-Space Clipping



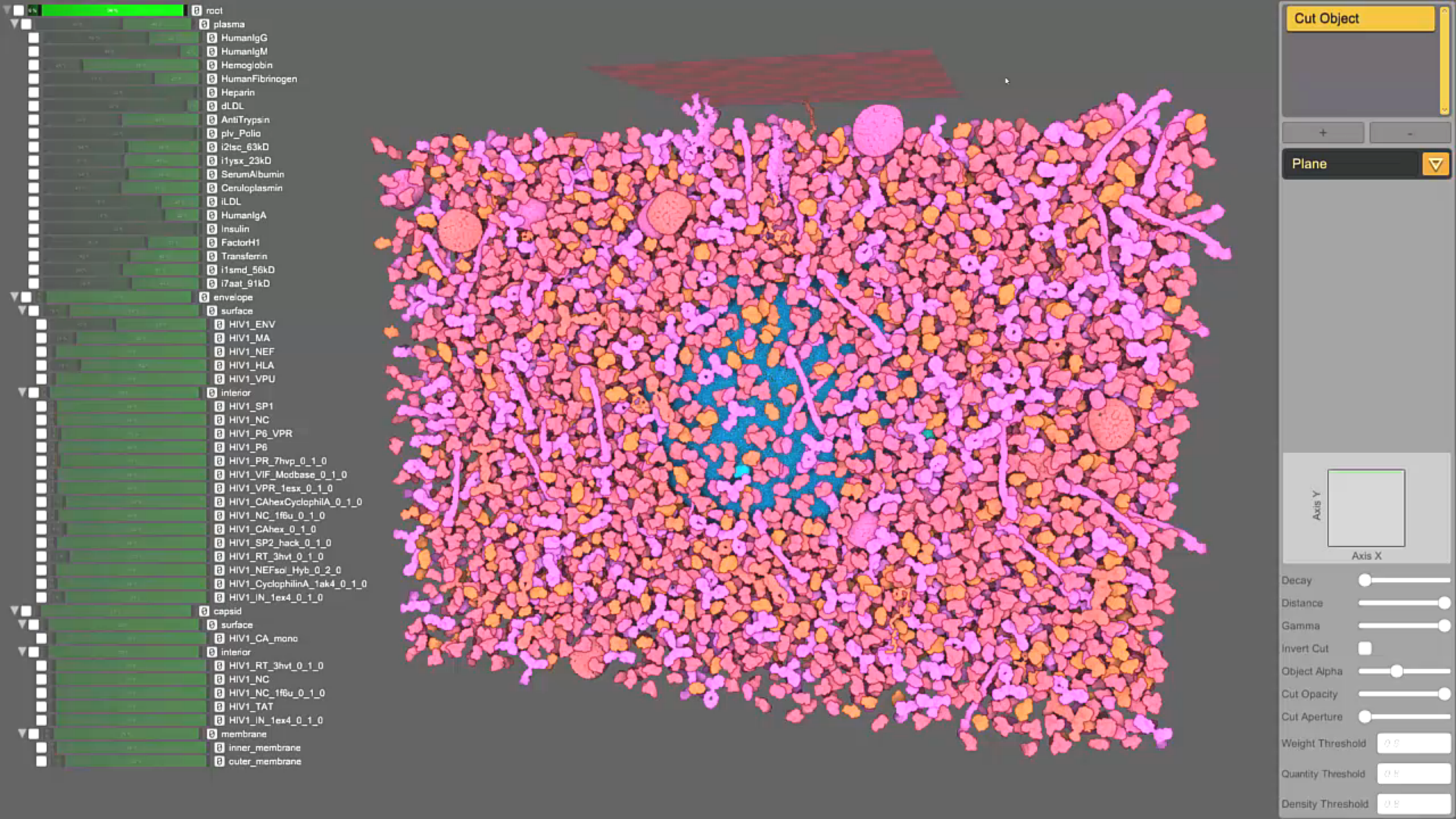


Uniform clipping

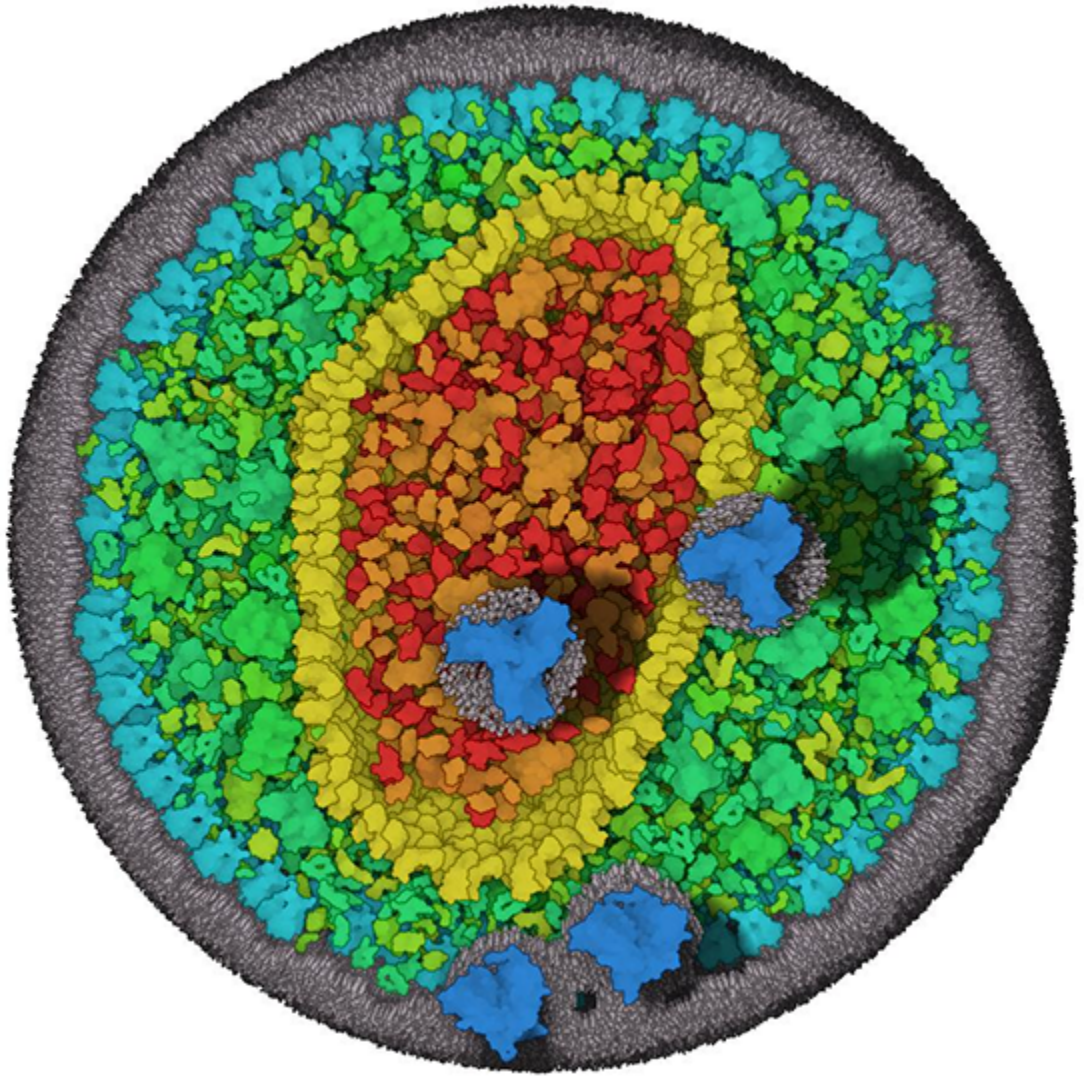


Aperture-based clipping

2D distance map


root
plasma
HumanIgG
HumanIgM
Hemoglobin
HumanFibrinogen
Heparin
dLDL
AntiTrypsin
plv_Polio
i2tsc_63kD
i1ysx_23kD
SerumAlbumin
Ceruloplasmin
iLDL
HumanIgA
Insulin
FactorH1
Transferrin
i1smd_56kD
i7aat_91kD
envelope
surface
HIV1_ENV
HIV1_MA
HIV1_NEF
HIV1_HLA
HIV1_VPU
interior
HIV1_SP1
HIV1_NC
HIV1_P6_VPR
HIV1_P6
HIV1_PR_7hvp_0_1_0
HIV1_VIF_Modbase_0_1_0
HIV1_VPR_1esx_0_1_0
HIV1_CAhexCyclophilA_0_1_0
HIV1_NC_1f6u_0_1_0
HIV1_CAhex_0_1_0
HIV1_SP2_hack_0_1_0
HIV1_RT_3hvt_0_1_0
HIV1_NEFsol_Hyb_0_2_0
HIV1_CyclophilinA_1ak4_0_1_0
HIV1_IN_1ex4_0_1_0
capsid
surface
HIV1_CA_mono
interior
HIV1_RT_3hvt_0_1_0
HIV1_NC
HIV1_NC_1f6u_0_1_0
HIV1_TAT
HIV1_IN_1ex4_0_1_0
membrane
inner_membrane
outer_membrane
Cut Object
+
-
Plane
Axis Y
Axis X
Decay
Distance
Gamma
Invert Cut
Object Alpha
Cut Opacity
Cut Aperture
Weight Threshold
Quantity Threshold
Density Threshold

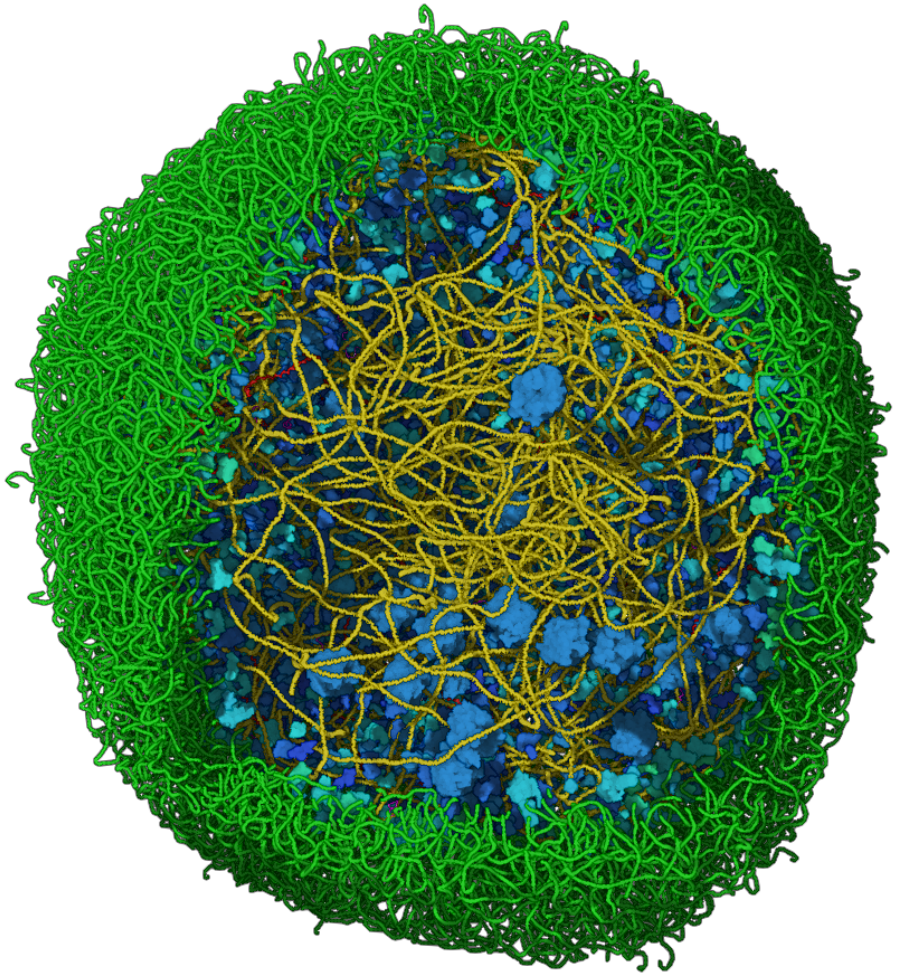
Contextual Anchoring

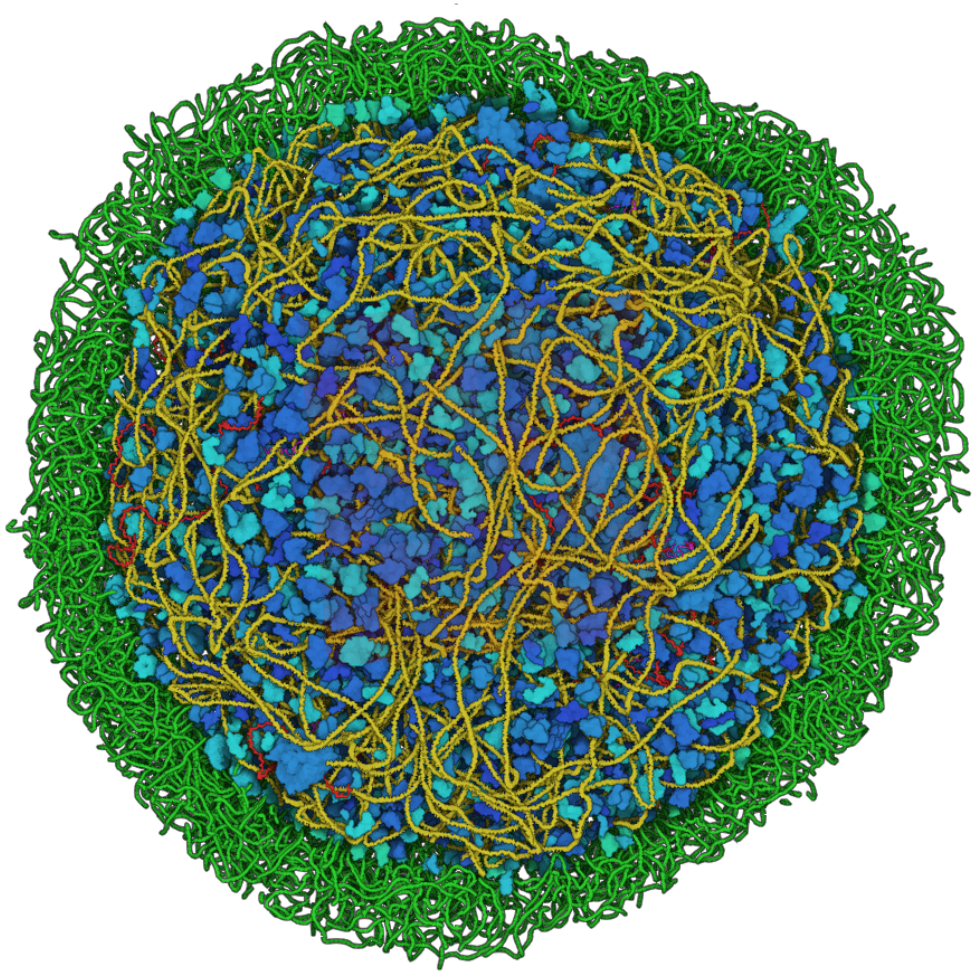


Using a depth bias to the occlusion query

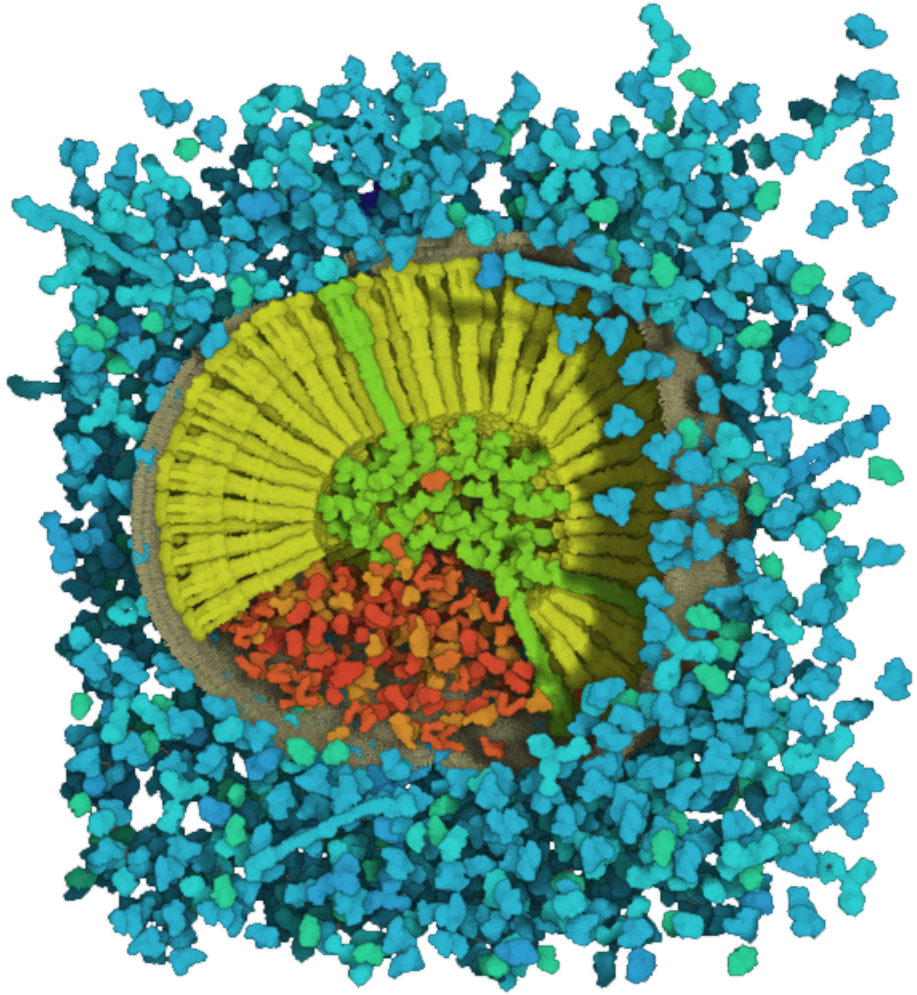
Results

Mycoplasma





Immature HIV



Performance

Some timings

- Intel Core i7-3930 CPU 3.2GHz, GeForce GTX Titan X 12GB RAM

- Object-space clipping:
  - **0.3 ms** to evaluate 236061 instances of the HIV + blood dataset without clipping
  - **0.5 ms** to slice the dataset in half
  - **0.6 ms** to clip it entirely

Some timings

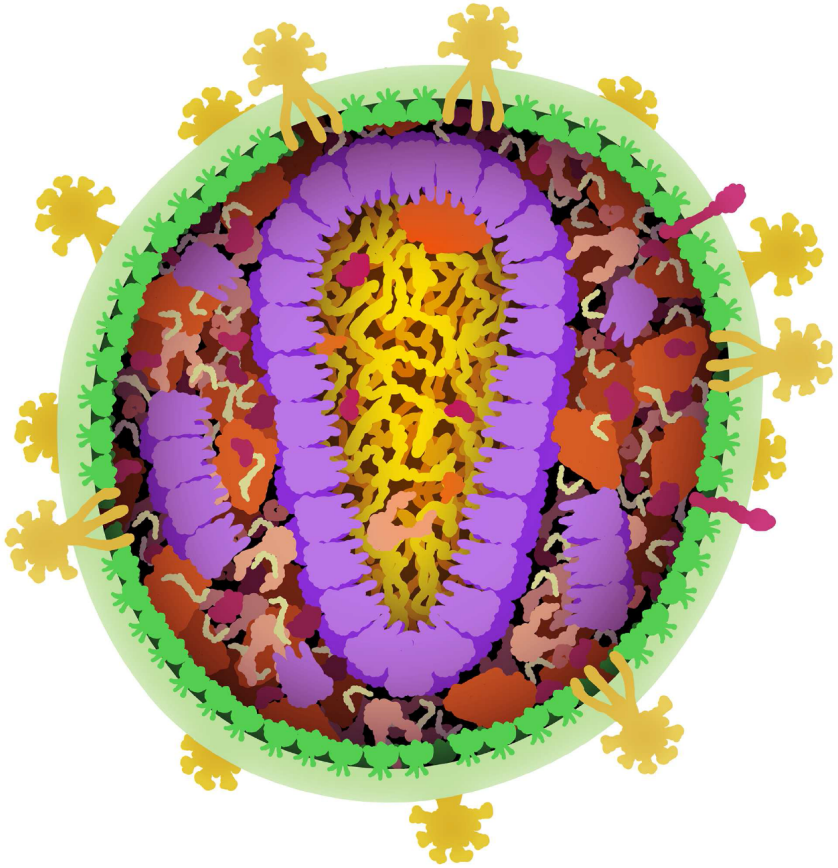
- Intel Core i7-3930 CPU 3.2GHz, GeForce GTX Titan X 12GB RAM

- View-space clipping (512x512 resolution):
  - **0.07 ms** to render the depth-stencil mask with 12142 instances (HIV proteins)
  - **0.57 ms** to compute 223919 occlusion queries (blood proteins + lipid residues)
  - **0.15 ms** to add the aperture effect

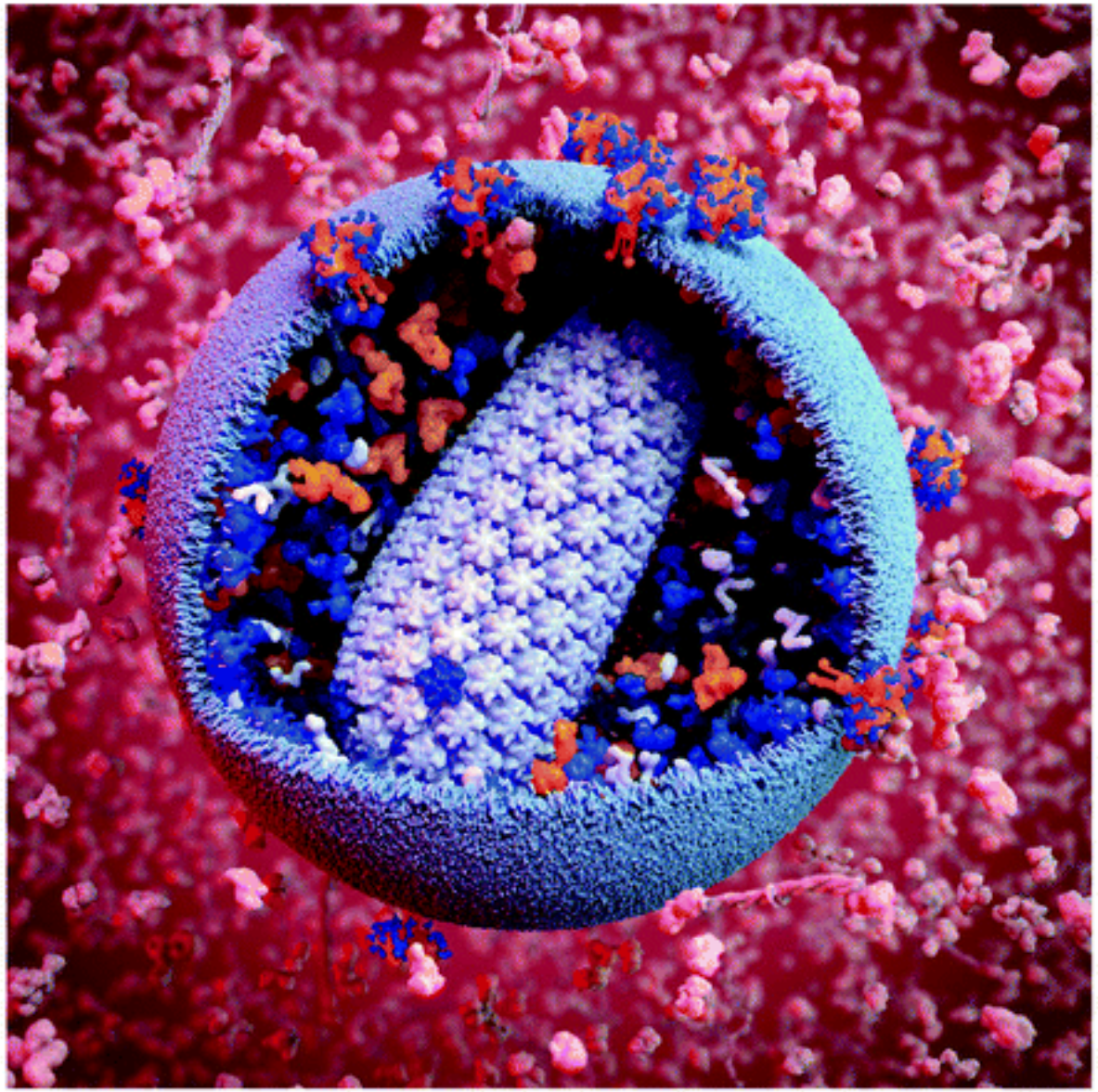
Conclusions

Using Instancing for Solving Visibility

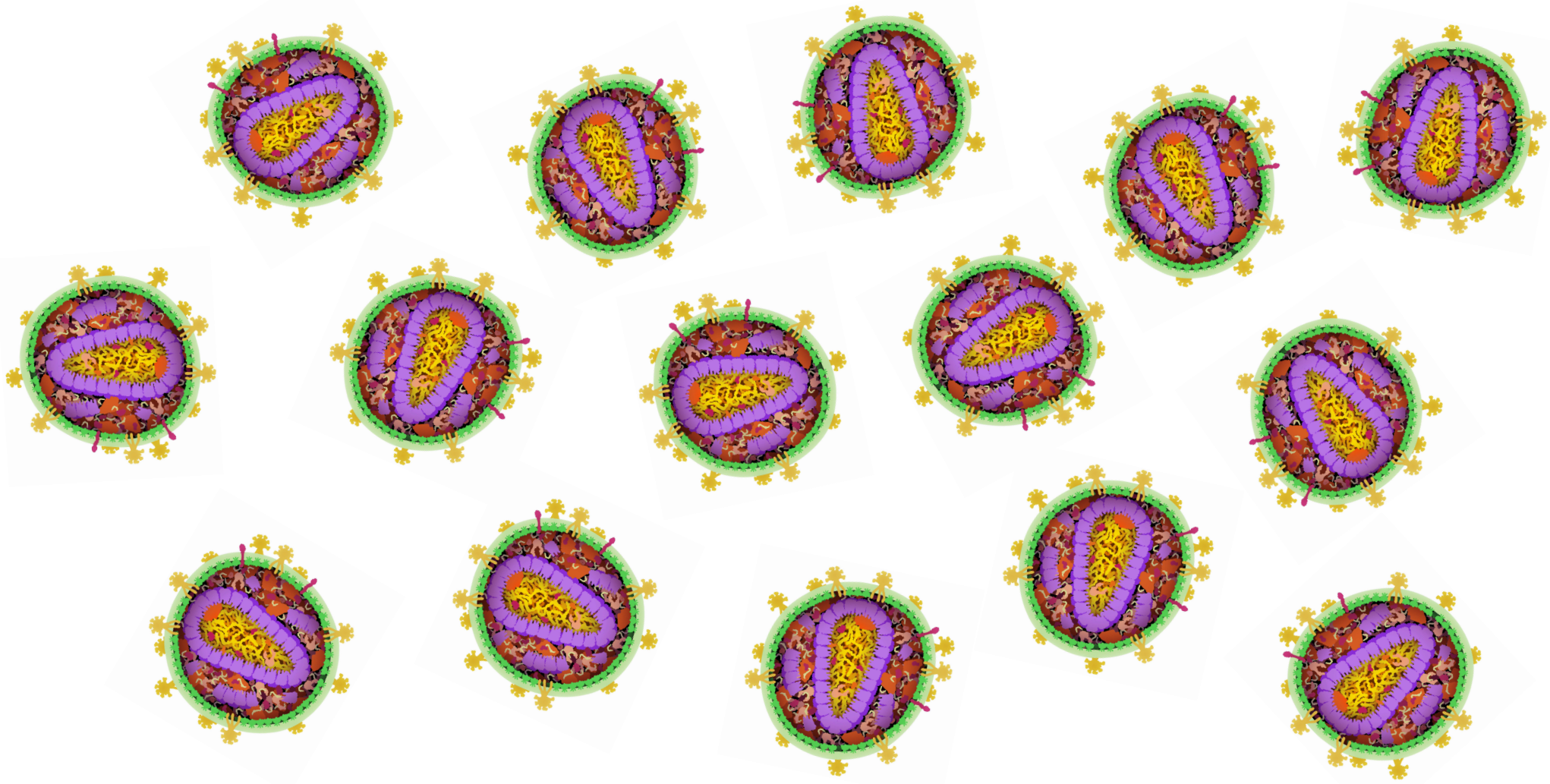
Using Instancing for Solving Visibility



Using Instancing for Solving Visibility



Using Instancing for Solving Visibility

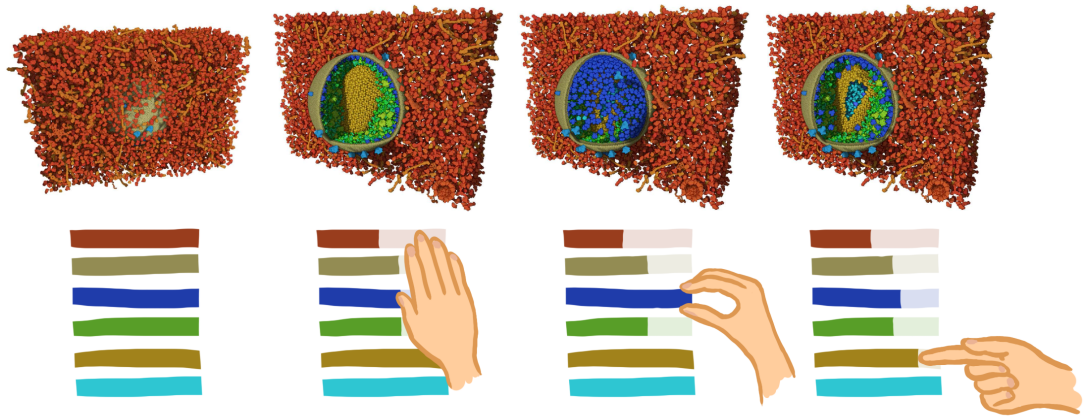


User feedback

- Biomedical illustrator: very useful
- Expert in molecular biology and visualization: enjoyed greatly, additional tools such as ghosting, were asked for.

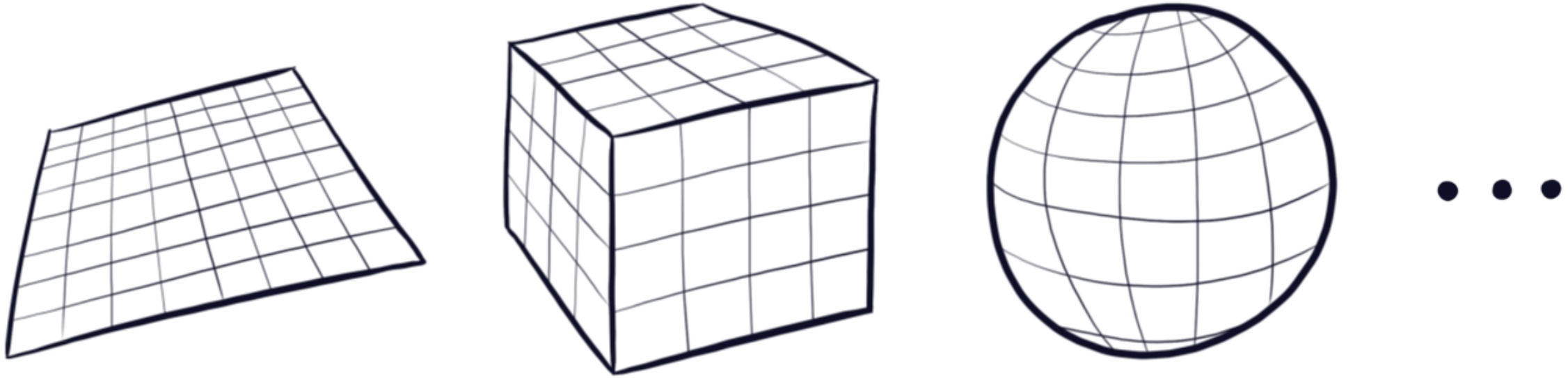
Thank you for your attention!

mindek@cg.tuwien.ac.at



CellView is free to use https://github.com/illvisation/cellVIEW

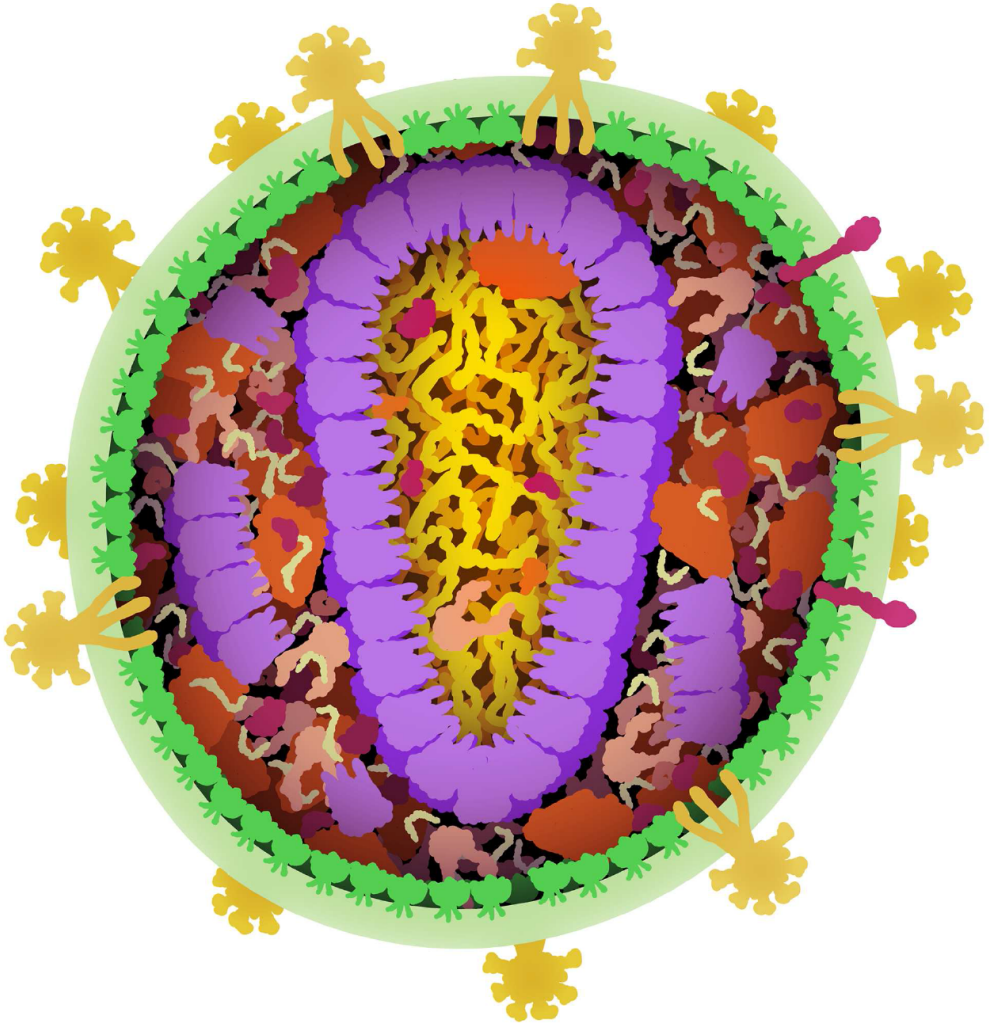
Implicit Clipping Objects



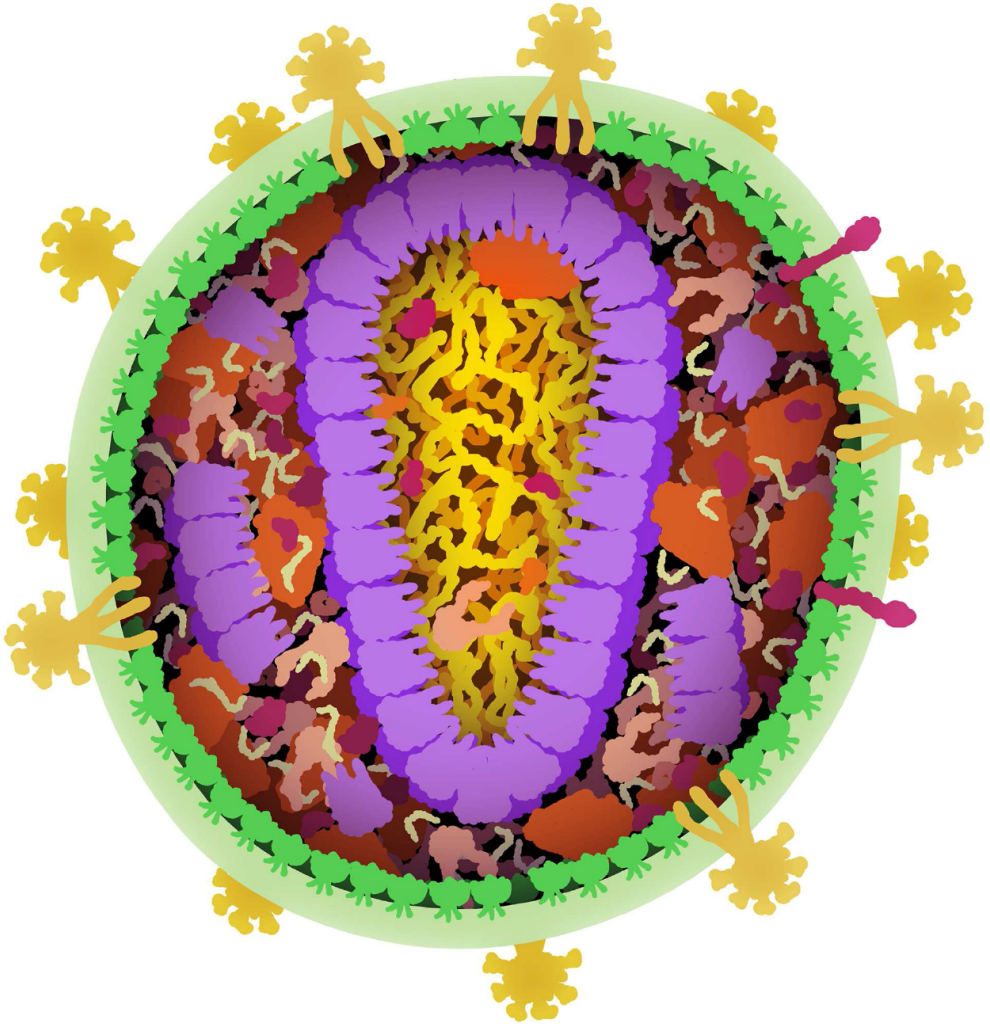
Mesoscopic Molecular Data

number of types << number of instances

Molecular Illustration



Which of these proteins are visible?



Cutaway Views