

# CS 526 Computer Graphics II

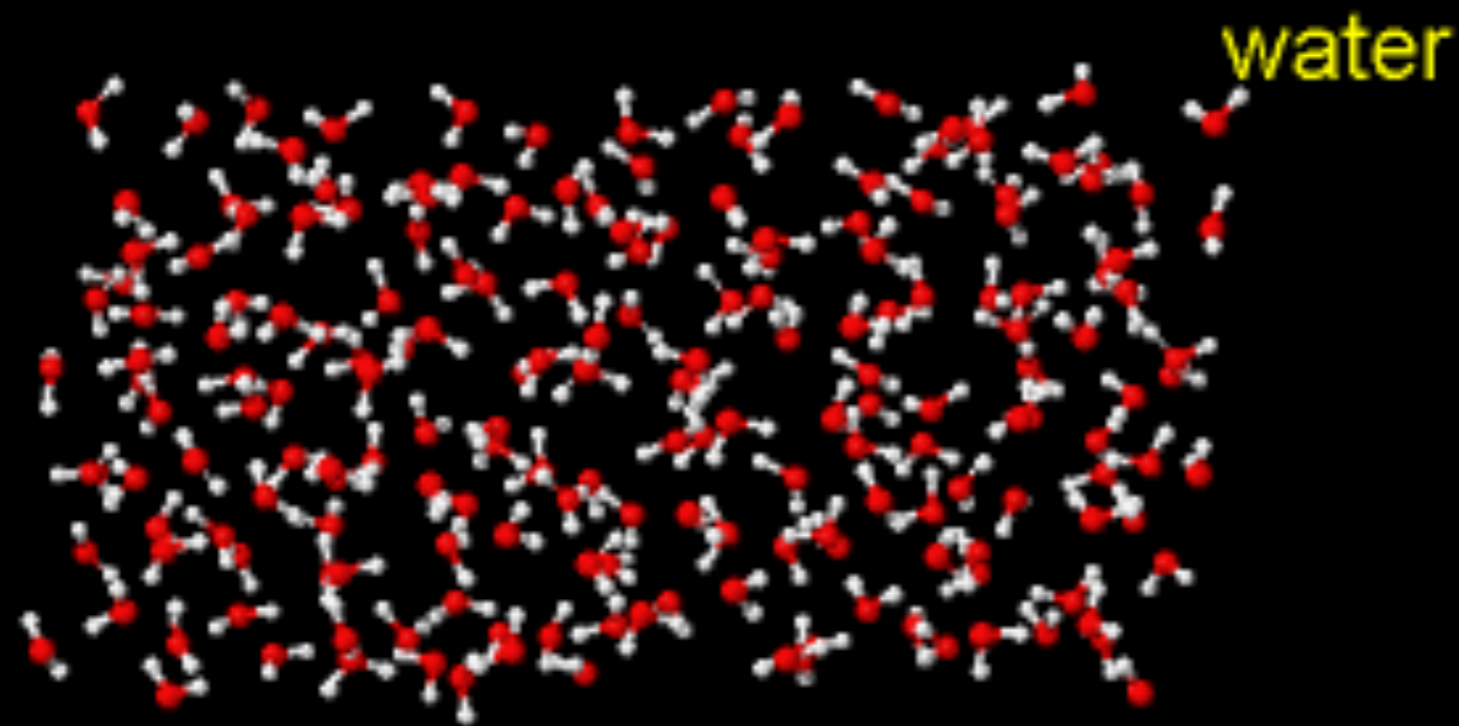
## Visualization in VR — Application to molecular vis

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UIC CS

# VR for Materials Science

Build better materials by studying the properties of matter at the **molecular** level



<http://biomodel.uah.es/agua/index.htm>

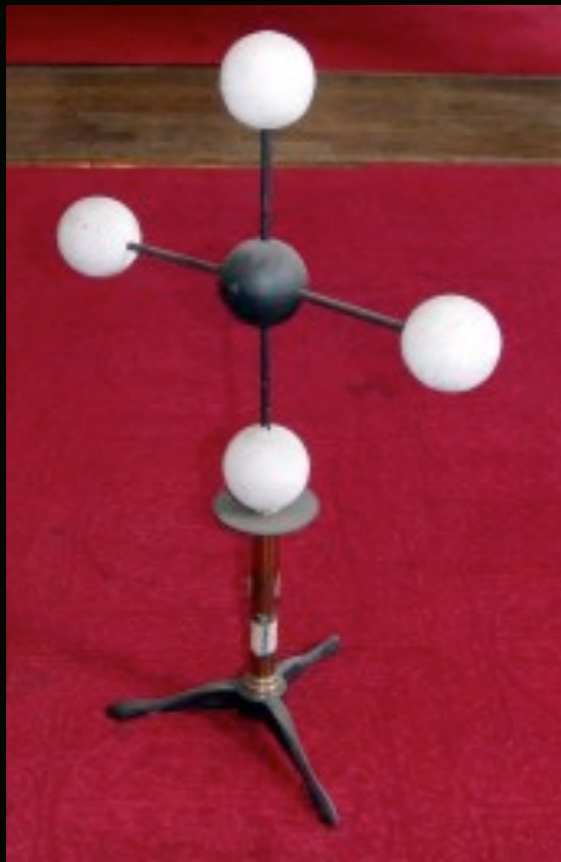
Chevy volt



Photovoltaic  
materials

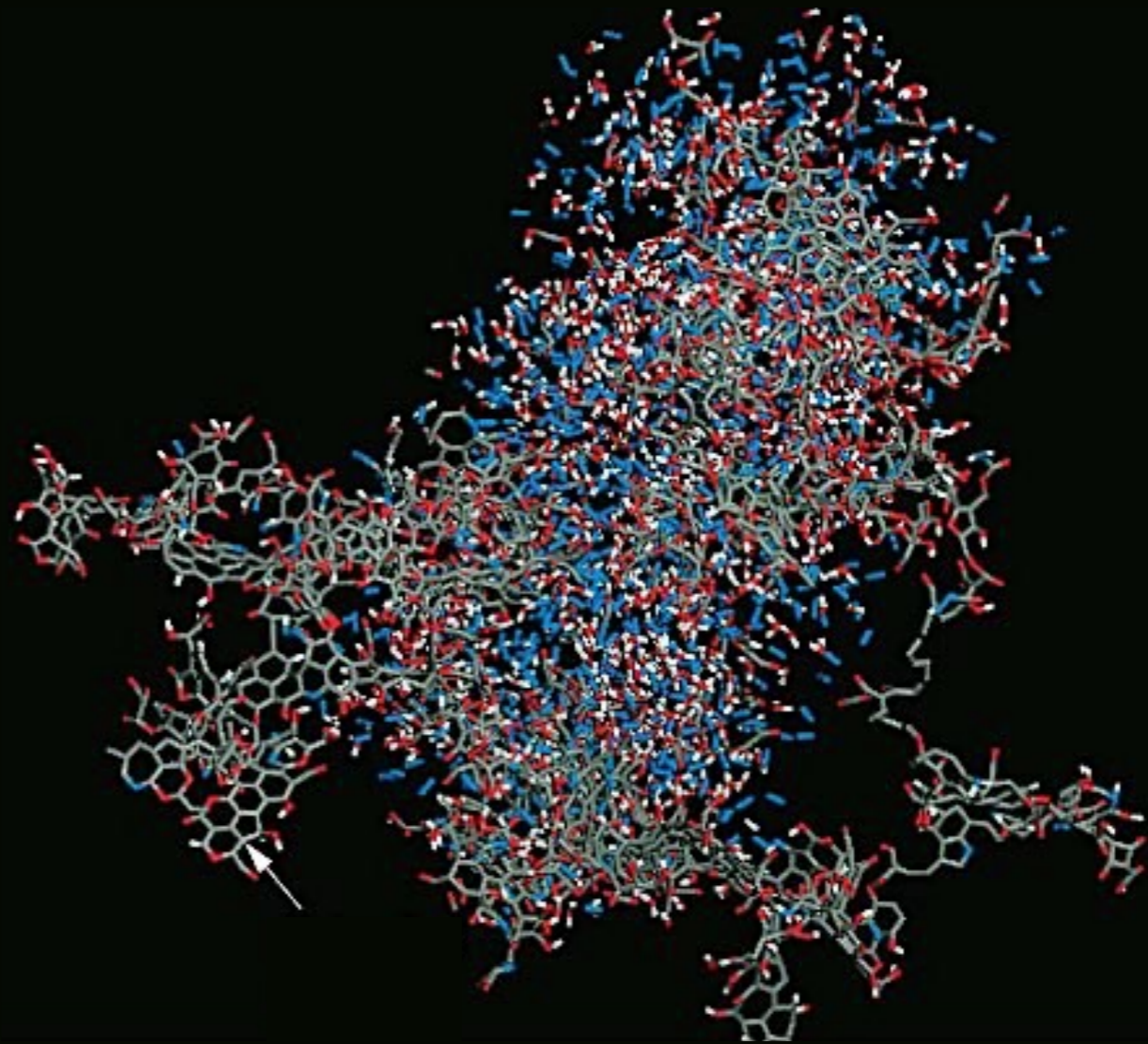
# Molecular Visualization

wikipedia



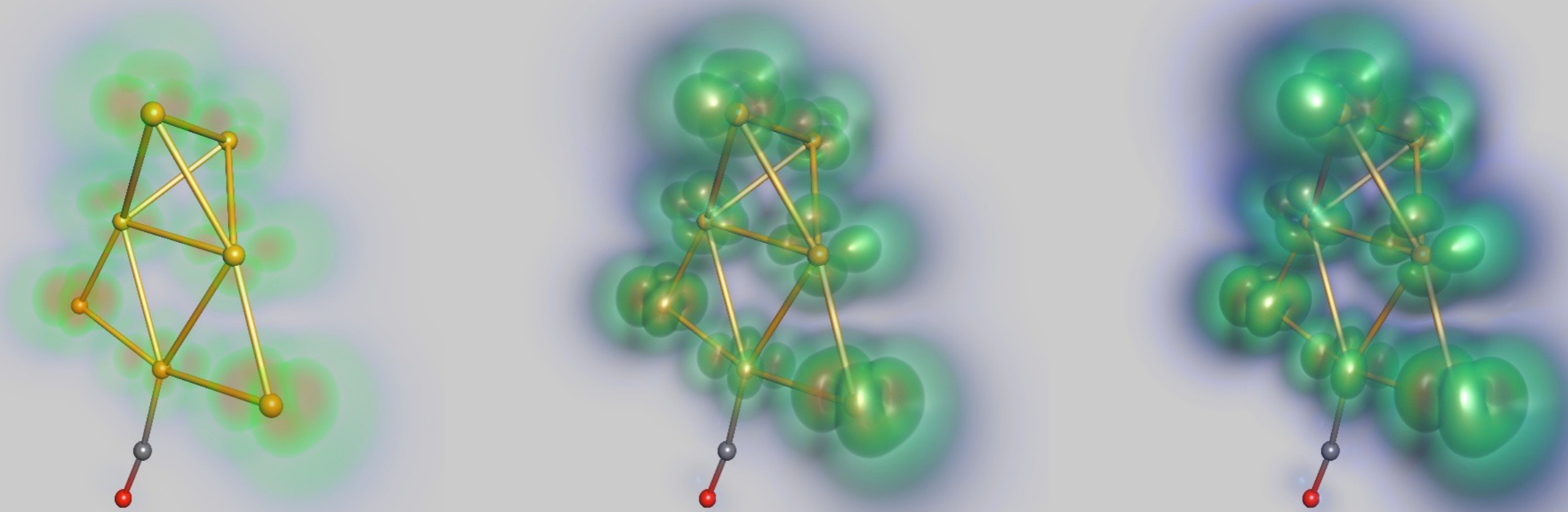
Hofmann's CH<sub>4</sub>  
model, 1865

<https://str.llnl.gov/JulAug12/maienschein.html>



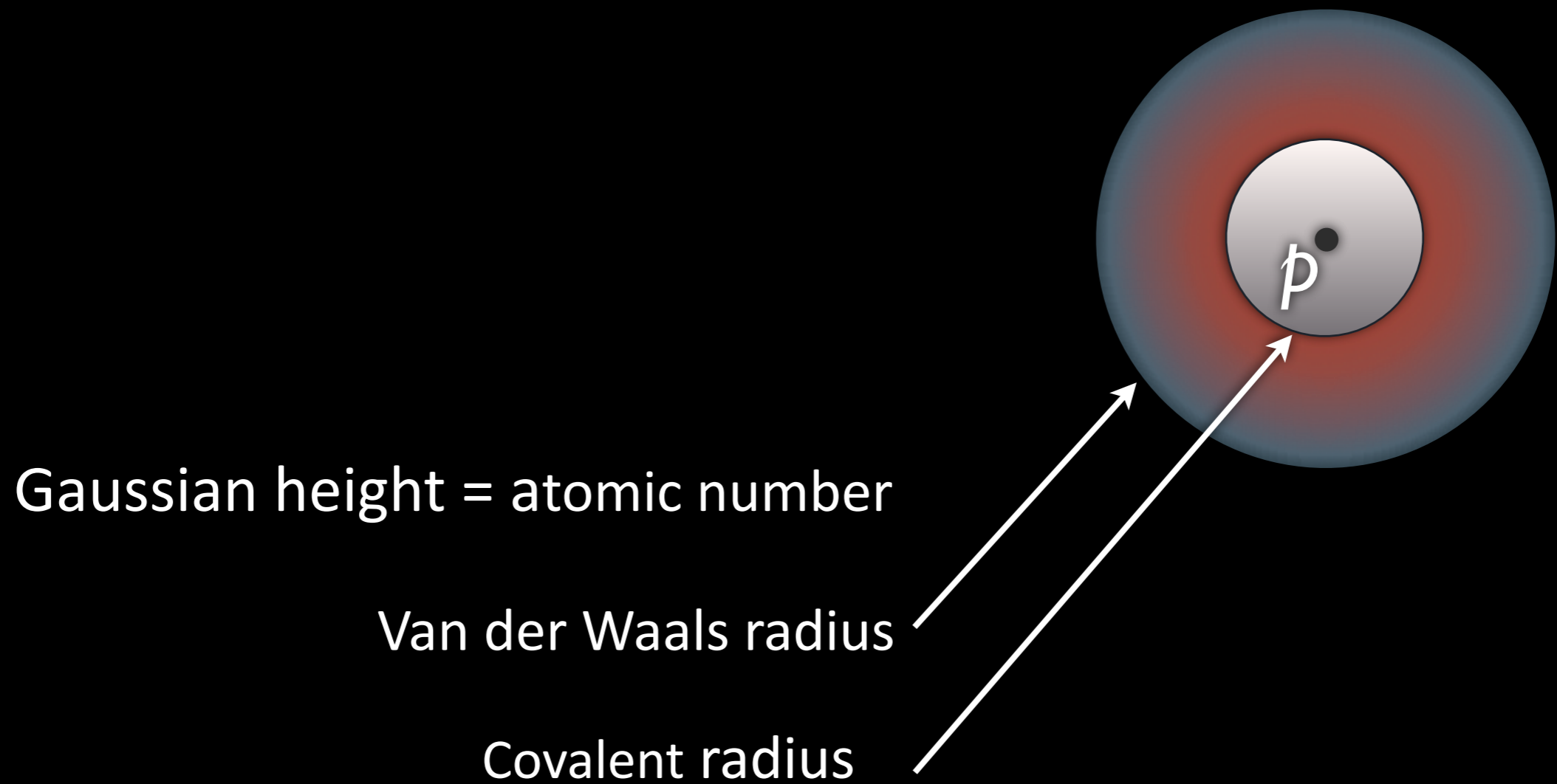
# Fuzzy boundary

Use electron density as a source of information when determining the boundary of materials

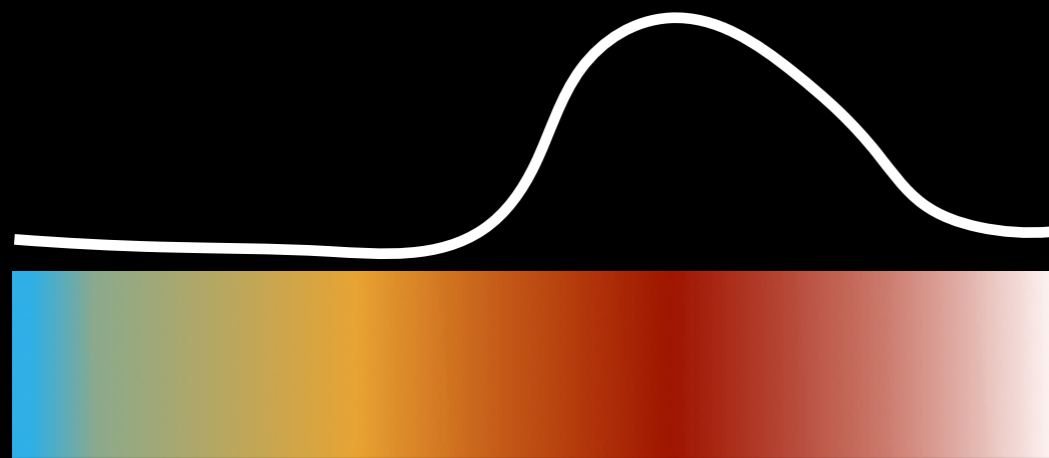


electron cloud  
opacity

# Approximate electron density

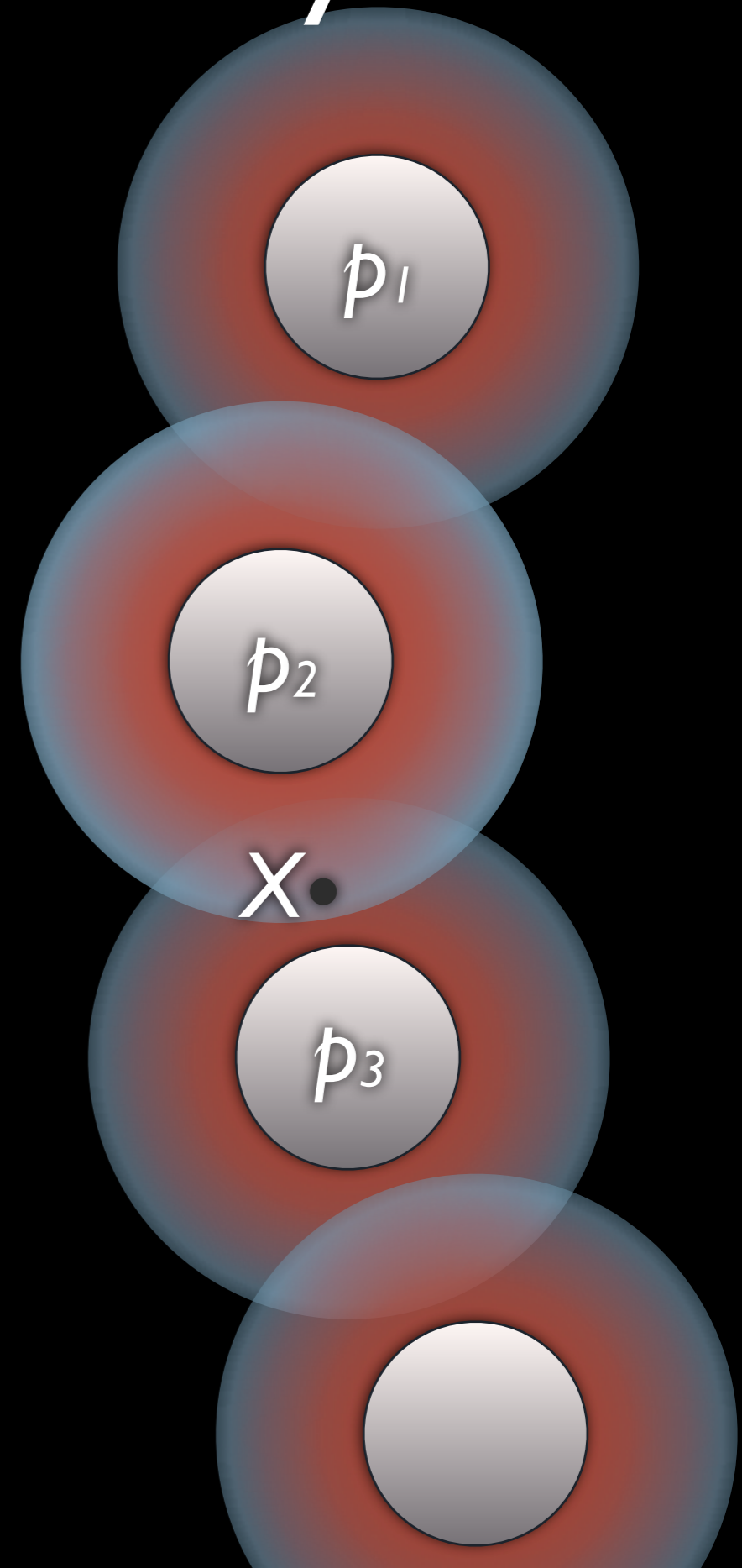


# Approximate electron density



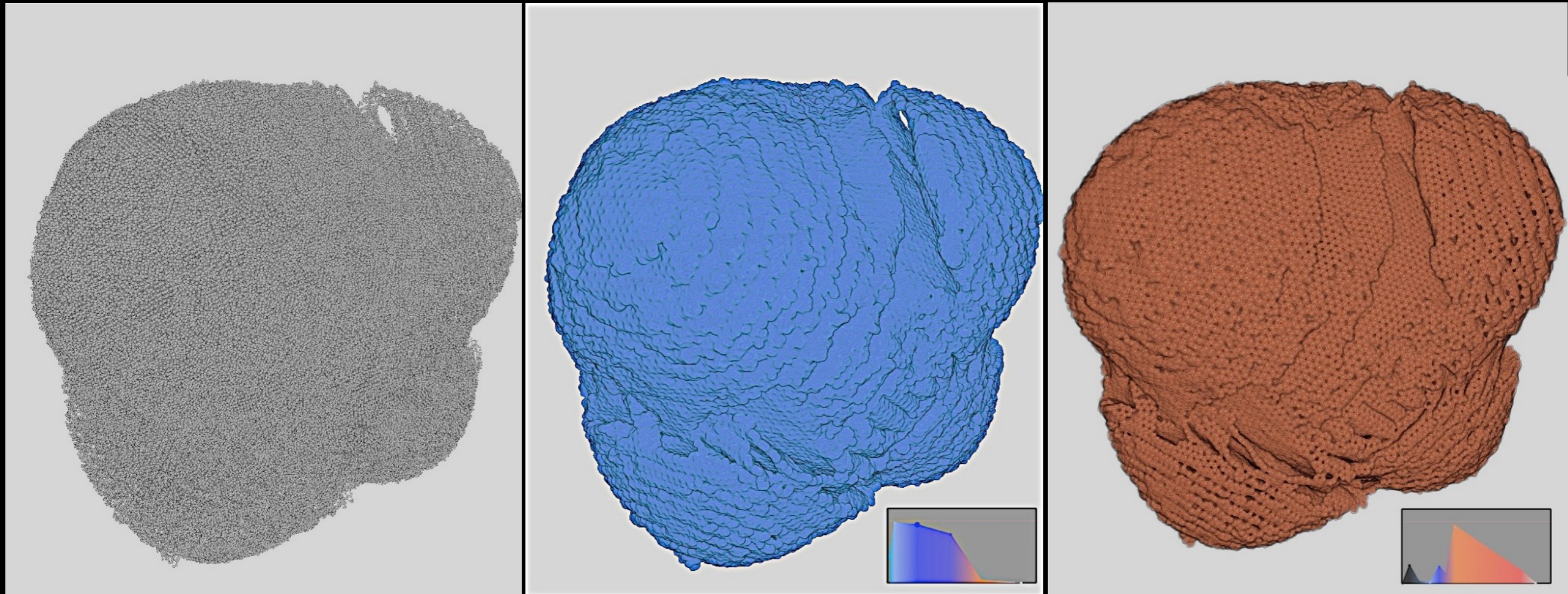
electronic  
density profile

color



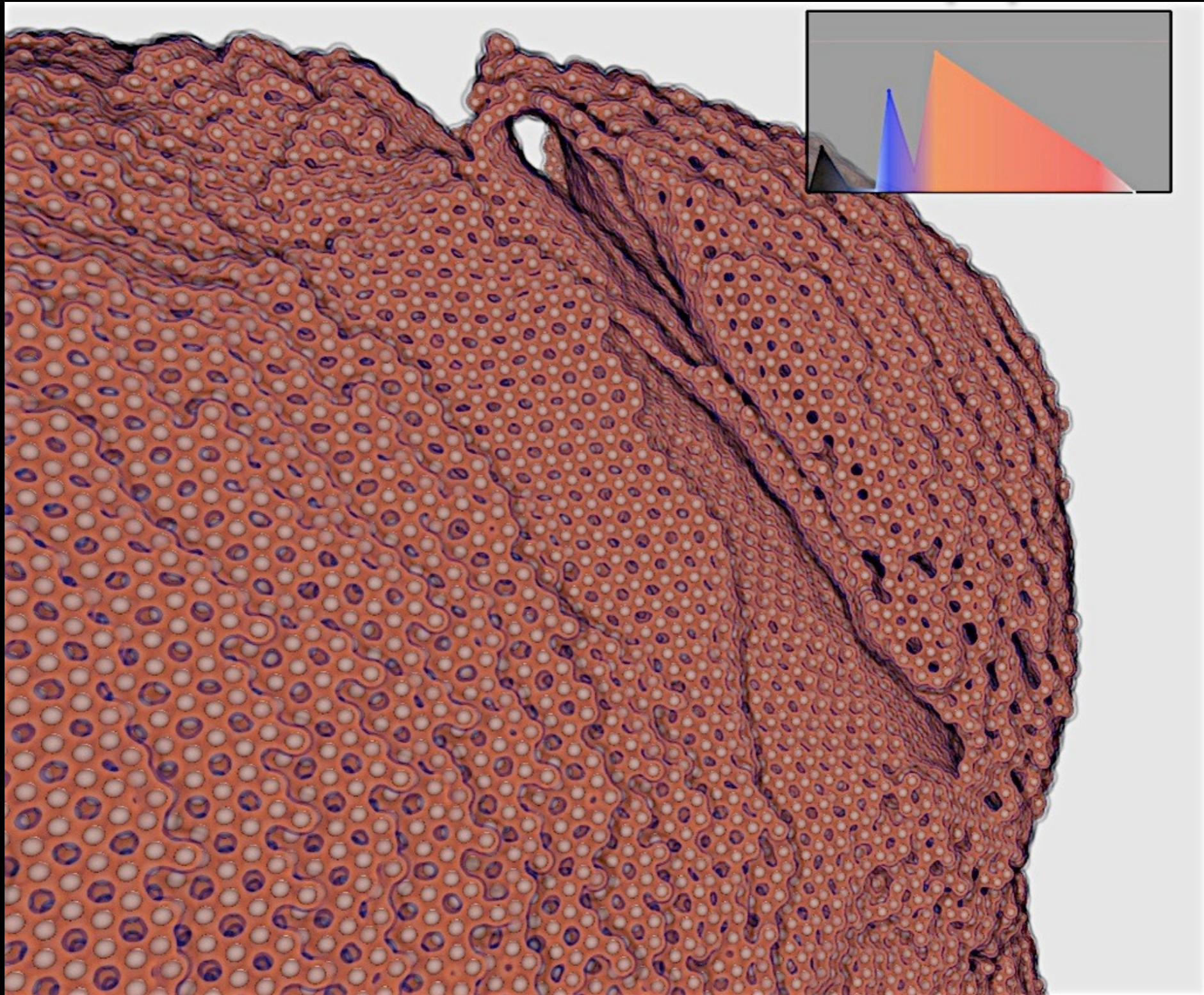


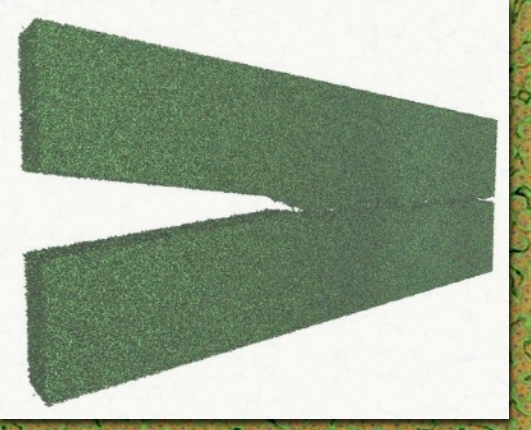
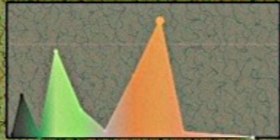
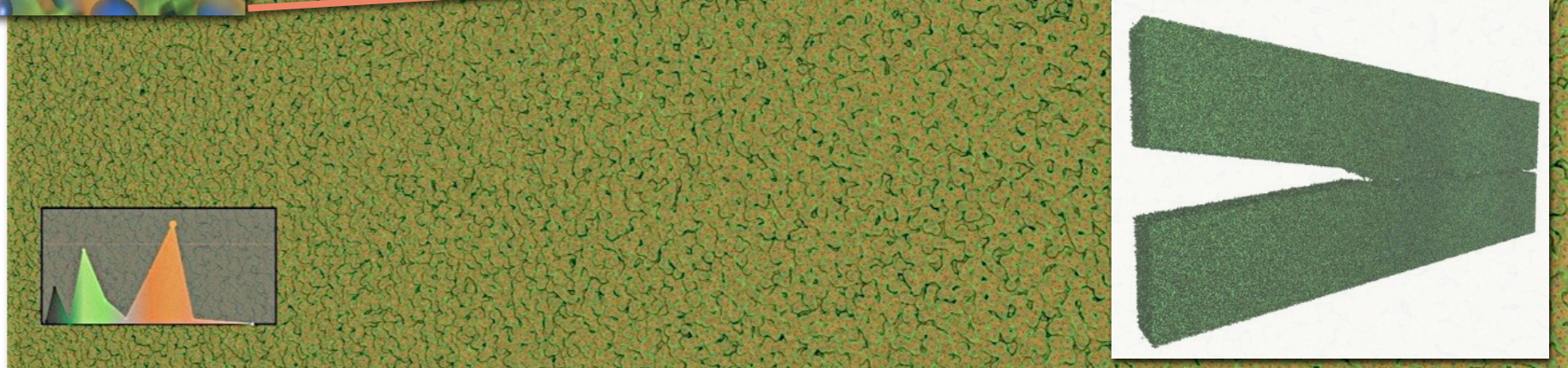
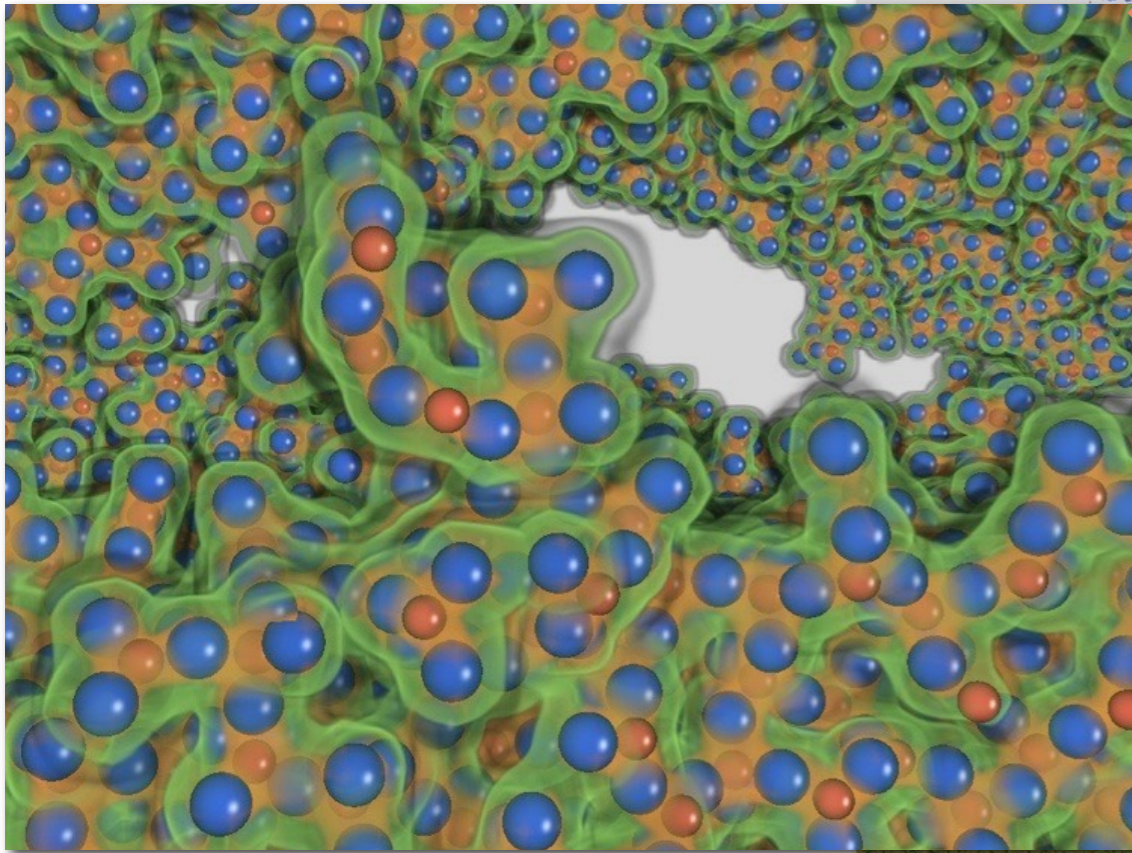
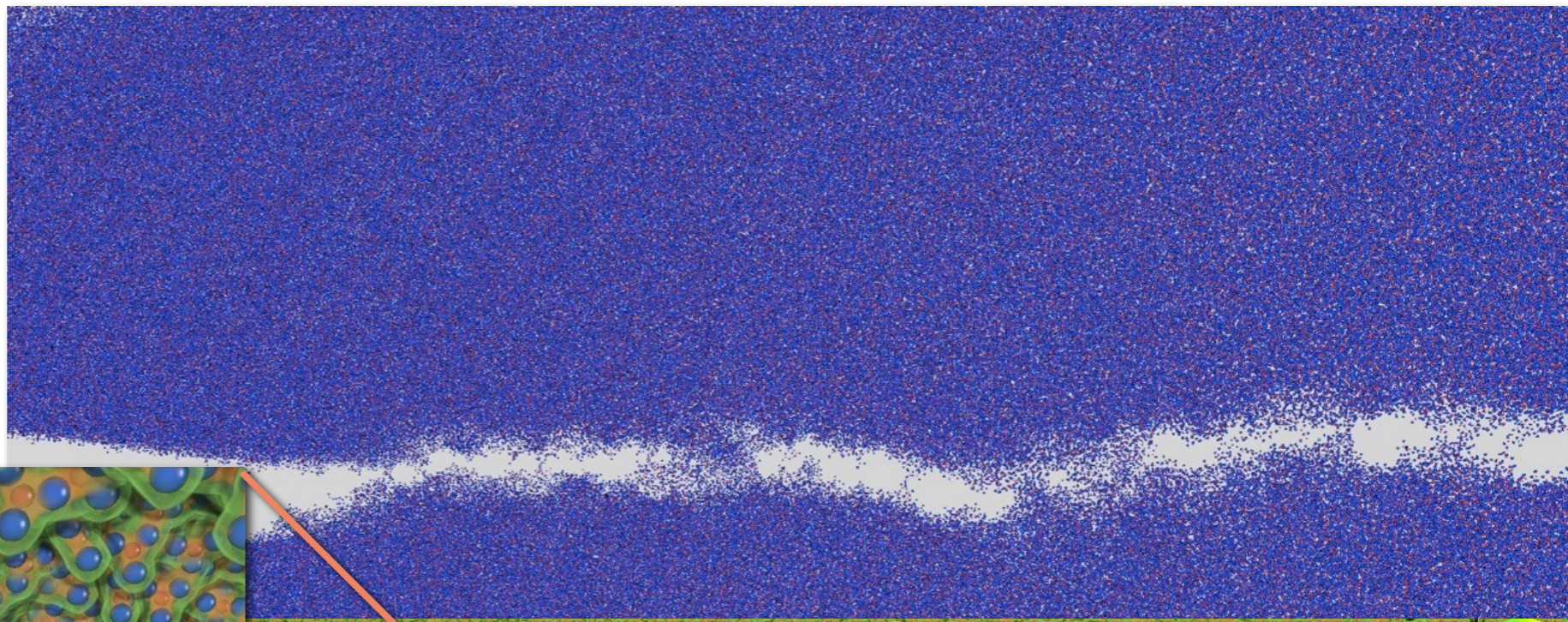
# Anode material (740K atoms)



# Anode material (740K atoms)

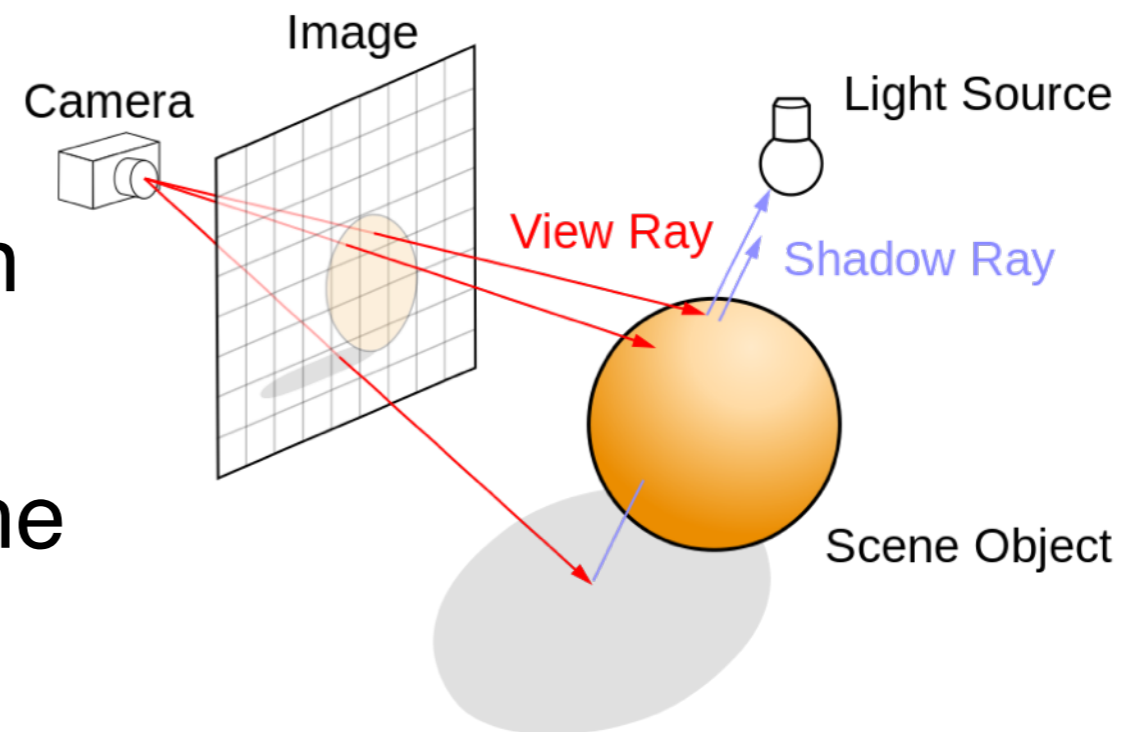
*Transfer function*





# Basic ray tracing

1. Create ray (one per pixel).
2. Intersect ray with objects in the scene.
3. Shade (compute color of the pixel)

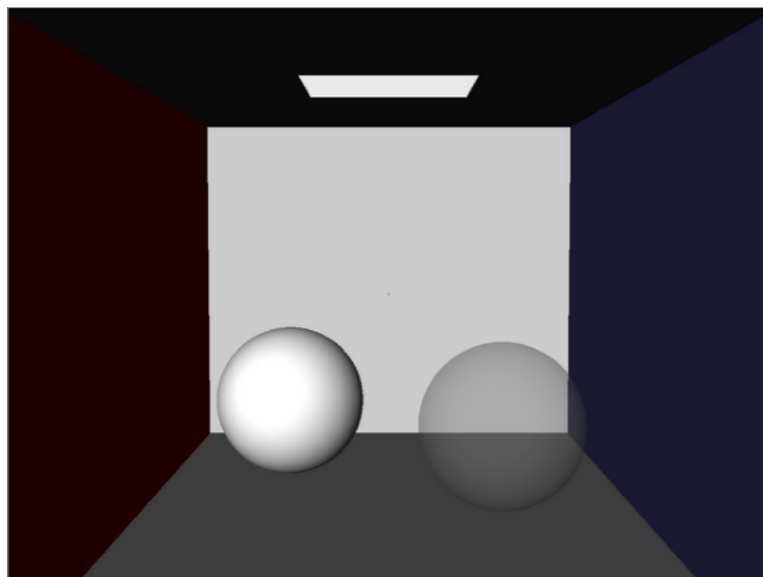


By Henrik - Own work, GFDL, <https://commons.wikimedia.org/w/index.php?curid=3869326>

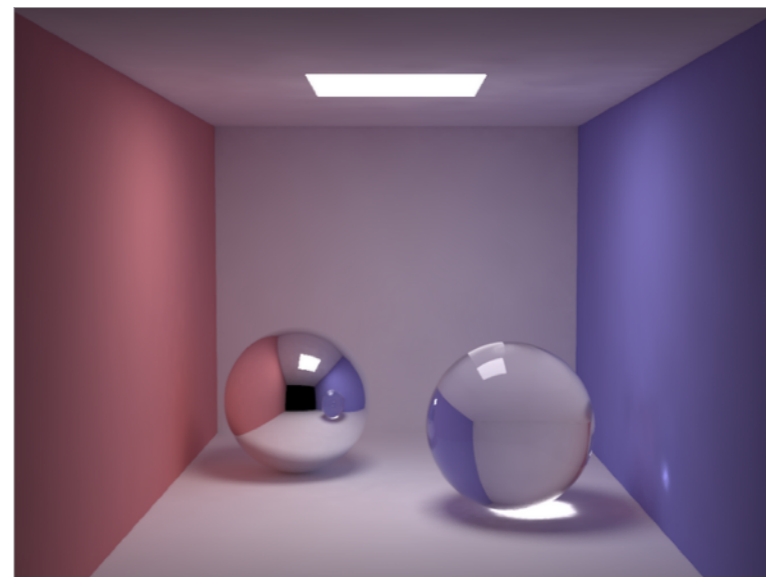
# Ray tracing vs. rasterization

- Illumination model:
  - Rasterization: local illumination – one primitive at a time.
  - Ray tracing: global illumination – one ray at a time (“easier” to determine global illumination effects).

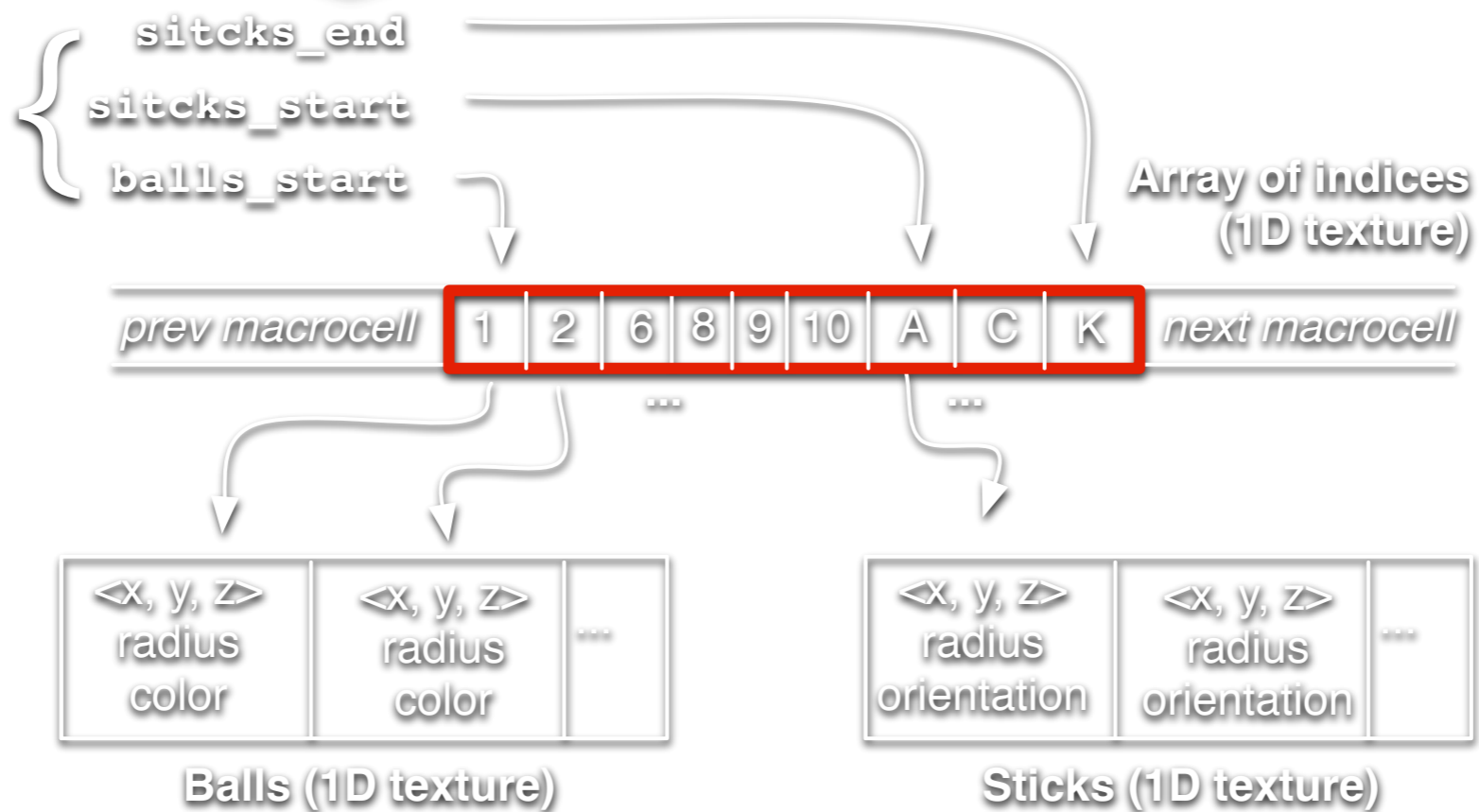
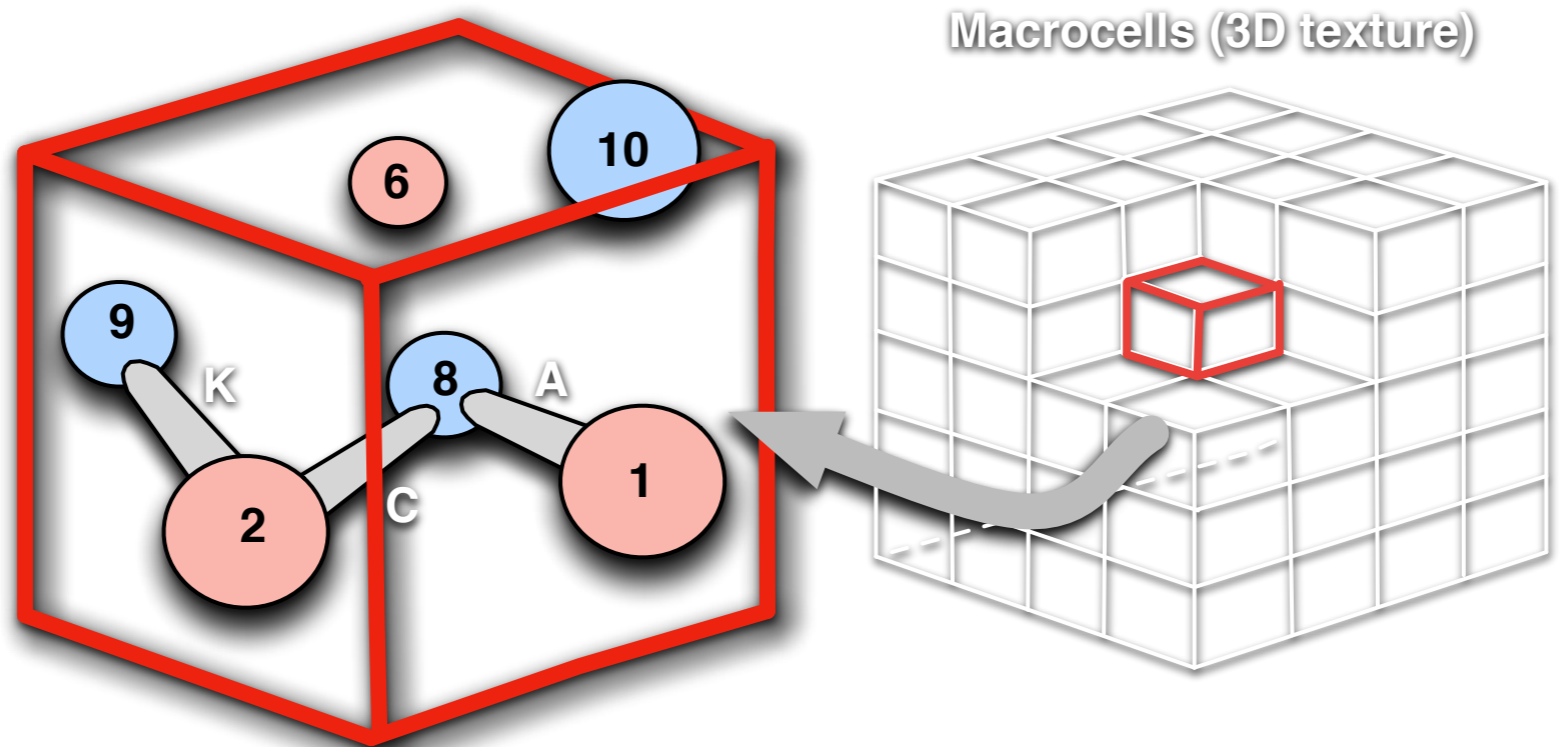
Rasterization

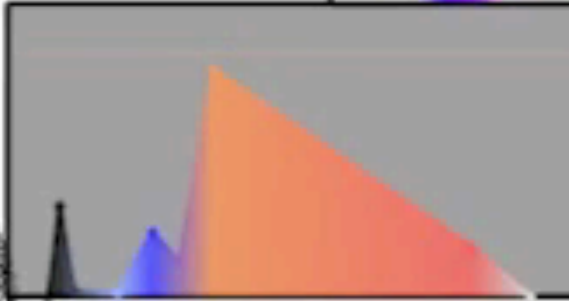
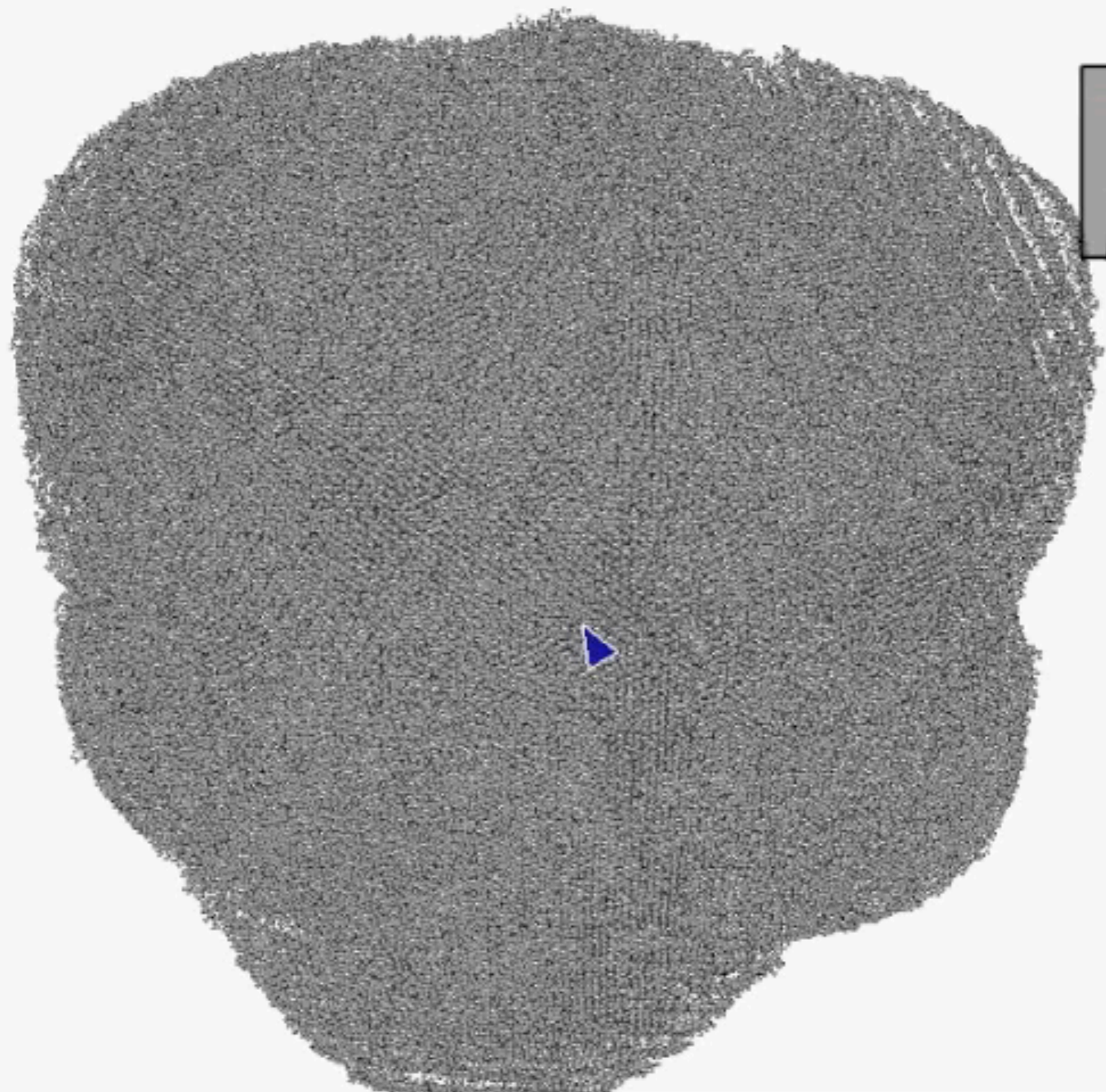


Ray tracing

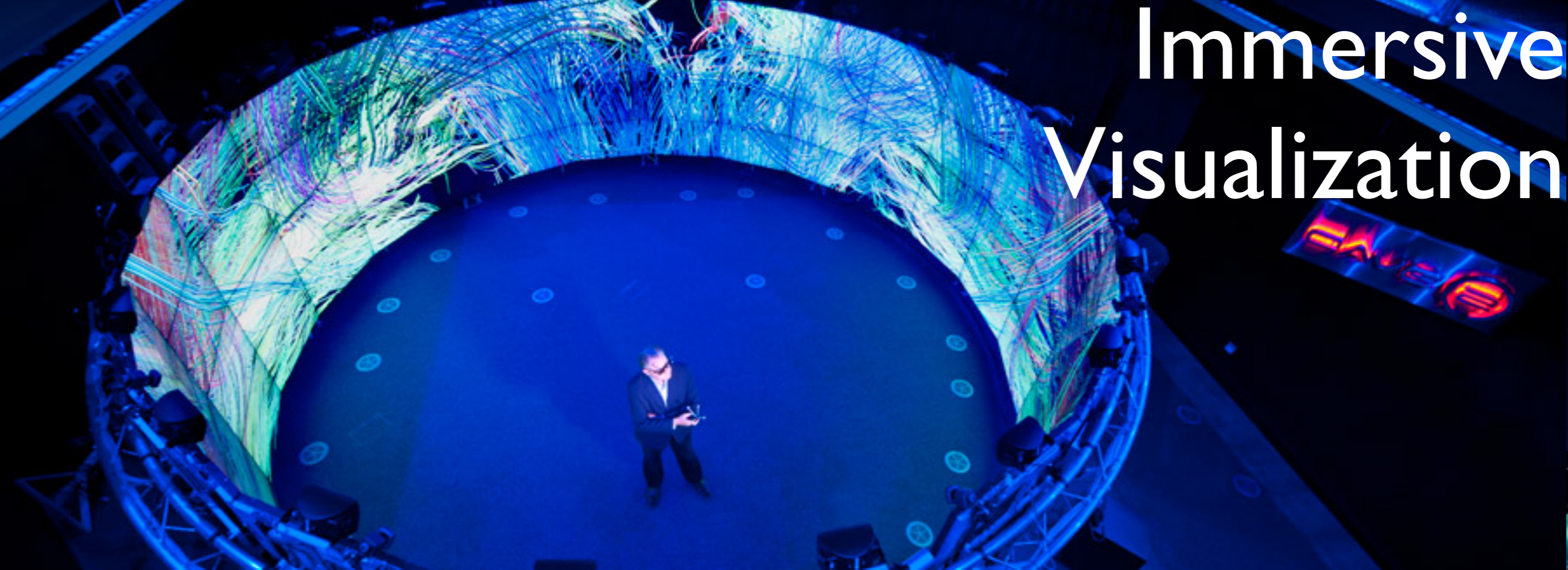


# GPU data model

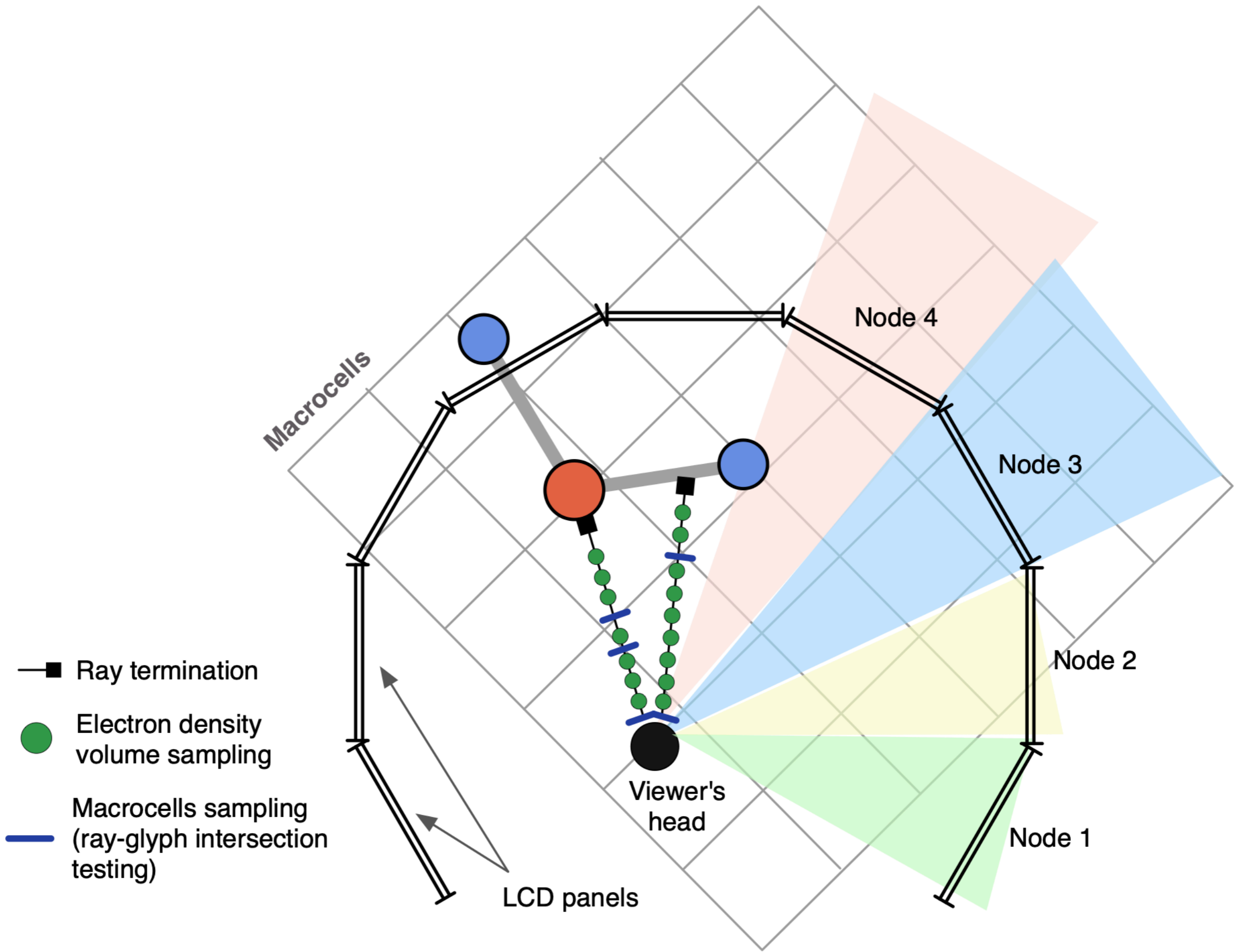




# Immersive Visualization







Macrocells

Node 4

Node 3

Node 2

Node 1

Viewer's head

LCD panels

# Stereoscopic projection

