جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology

VCC VISUAL COMPUTING CENTER

Nanovisualization

Ivan Viola

Motivation

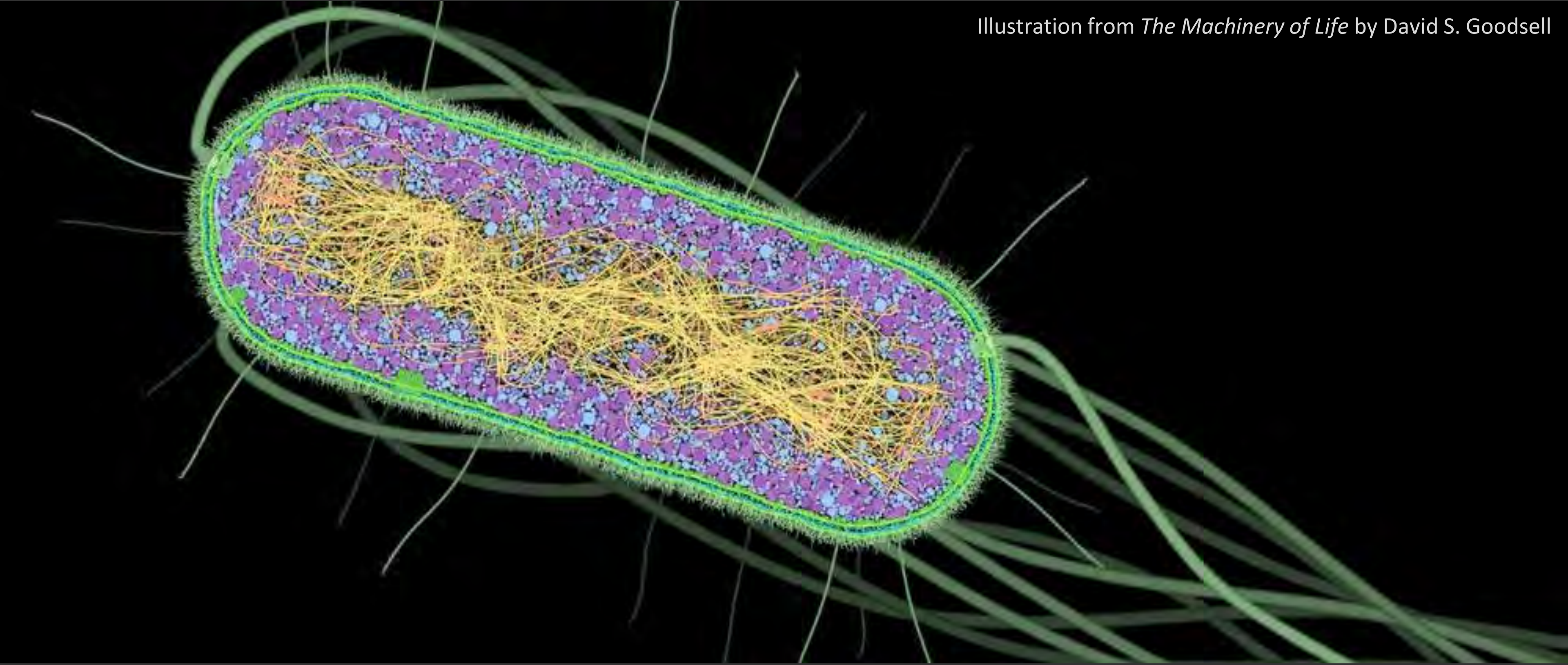
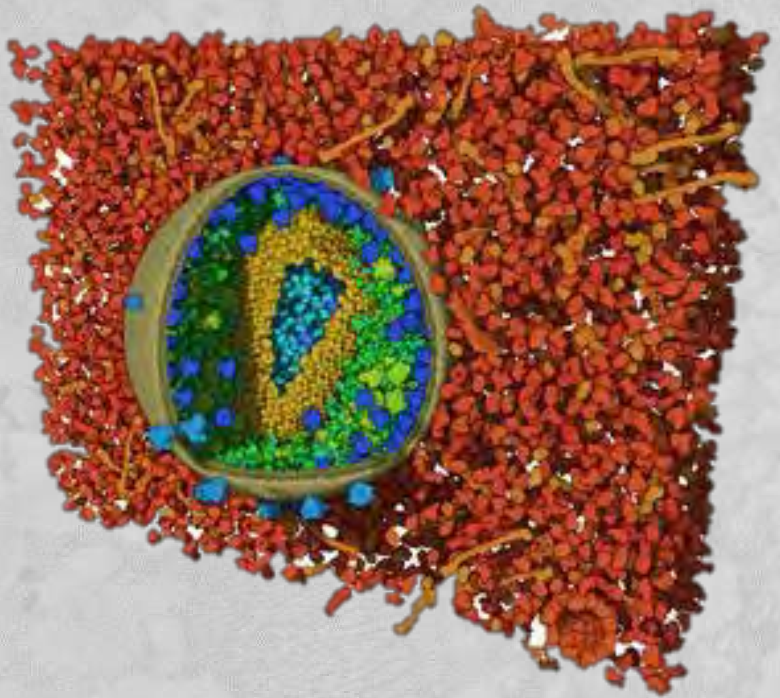


Illustration from *The Machinery of Life* by David S. Goodsell


SHOW CUT
root
HIV in Blood Plasma
Mesoscale modeling is used to study the molecular structure and interactions of large viruses and cells. These integrative models combine atomic information from structural biology with ultrastructural information from microscopy, using proteomic information as a bridge. This model includes a mature HIV virion surrounded by blood plasma, built with CellPack. These types of models are used by researchers to develop and test basic hypotheses about mesoscale structure and function. For instance, similar models of HIV were used to interpret fluorescence data that probed the distribution of envelope glycoproteins on the surface of the virus, which is important in recognition of the cells that the virus infects.
Reset Camera
EXPERT MODE
EXIT

Mission Statement

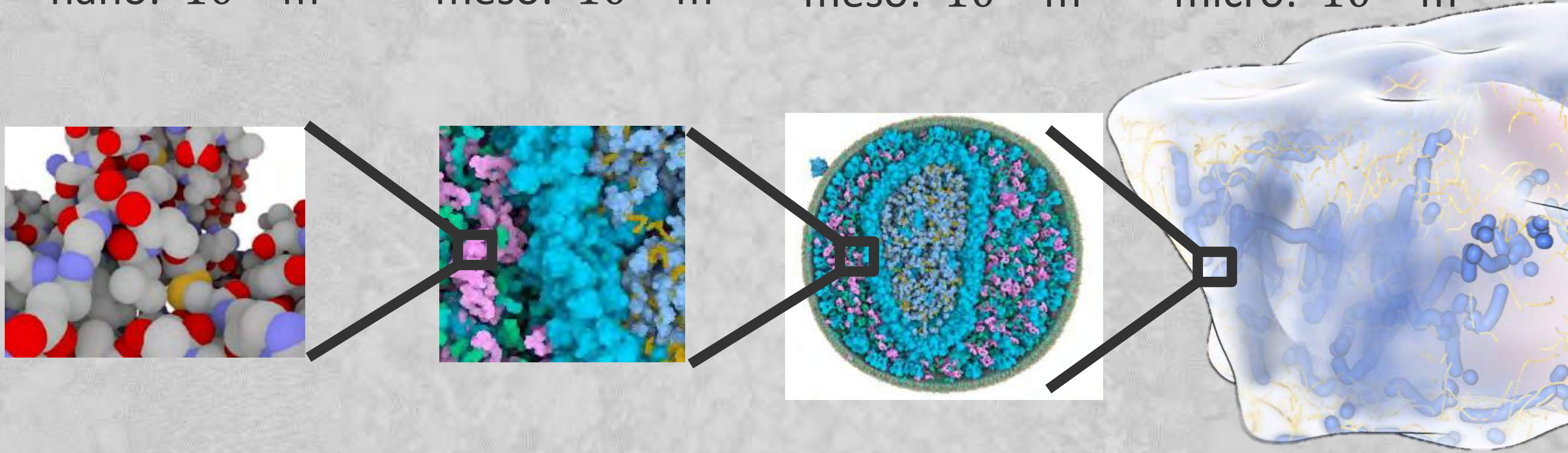


"Creating next-generation ***computer graphics*** *and* ***visualization*** *technology for depicting the life forms across all scales."*

Our Technology in Production

Scale between Cells and Atoms

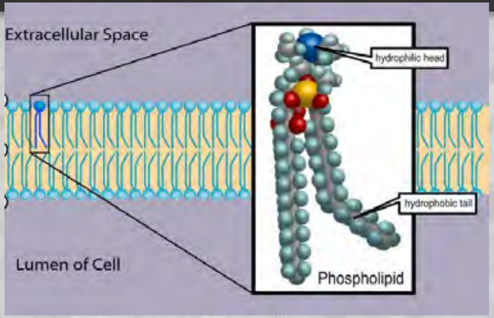
nano: 10^{-9}m meso: 10^{-8}m meso: 10^{-7}m micro: 10^{-6}m



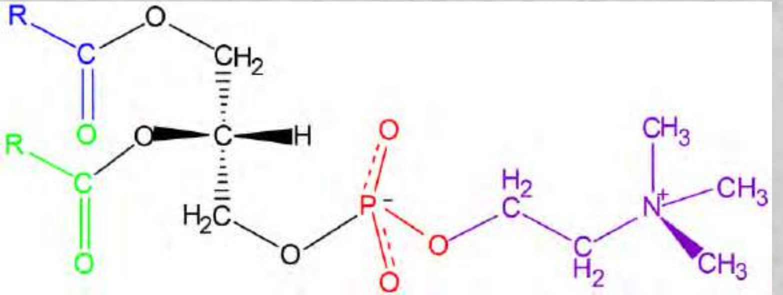
Chemistry 101: Atoms and Molecules

Molecules

- Atoms (118 chemical elements)
- Nucleus: protons and neutrons
- Orbit: electrons
- Bonds (covalent, ionic, disulfide, hydrogen)



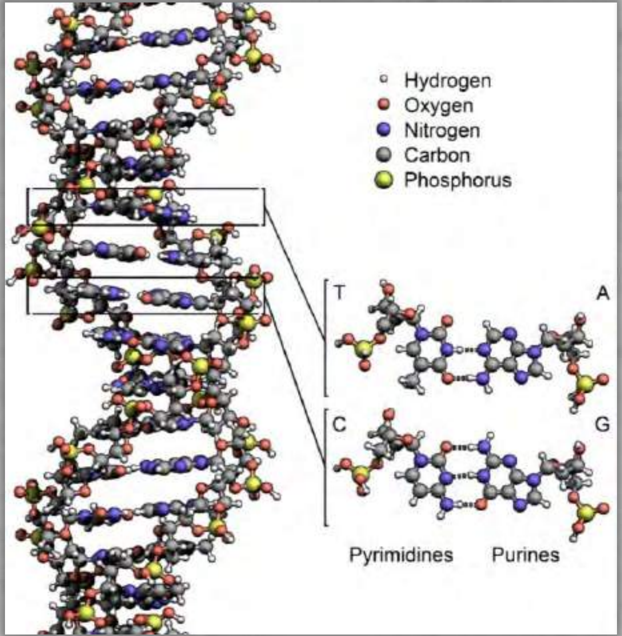
By Superscience71421 - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=53649846



http://en.wikipedia.org/wiki/Phospholipid

Chemistry 101: Nucleic Acids DNA RNA

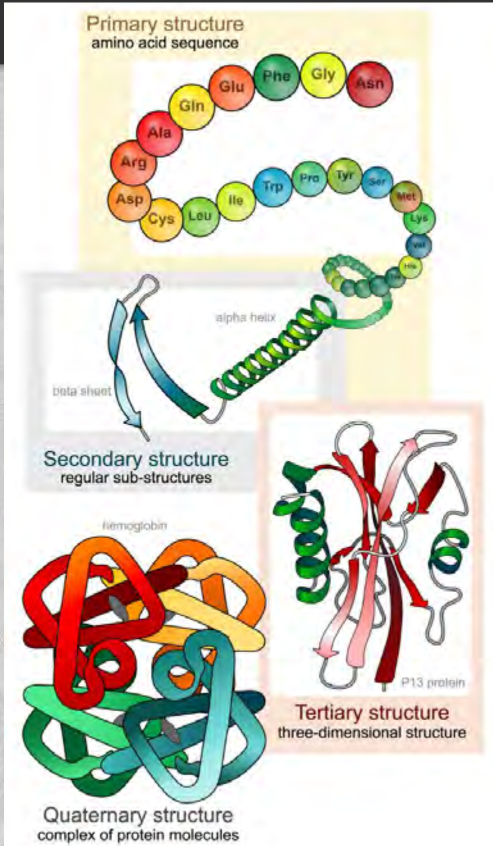
- DNA stores the “genetic code” - blueprint for proteins
- Chain of nucleotides
- Sugar backbone Desoxyribose
- Nucleobase Cytosine,Guanine, Adenine, Thymine/Uracil)
- Three nucleotides encode one amino acid



https://en.wikipedia.org/wiki/DNA

Chemistry 101: Proteins

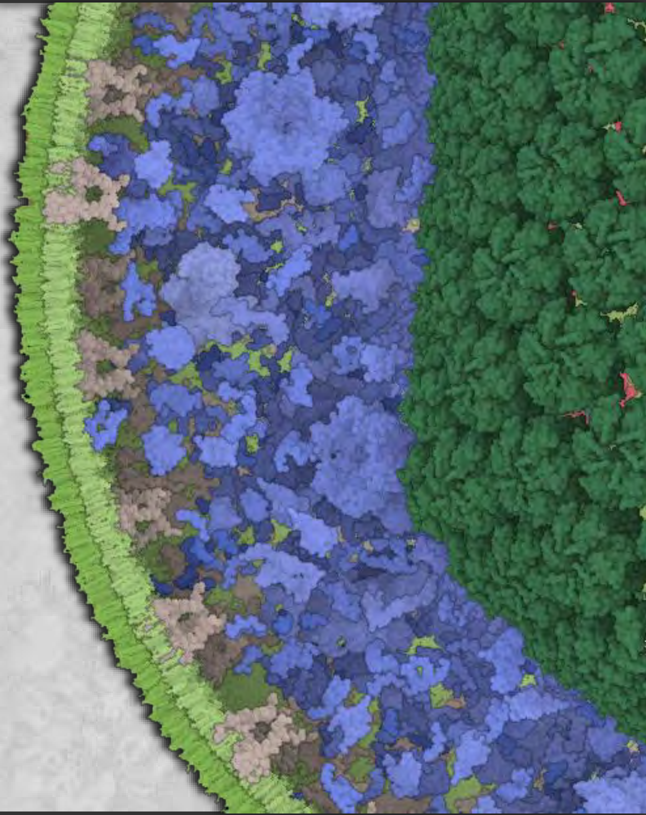
- Building blocks of the „machinery of life“
- Consist of amino acids
  - Linear chains that form a functional complex
  - Secondary structure (helix, sheet, turn, coil)



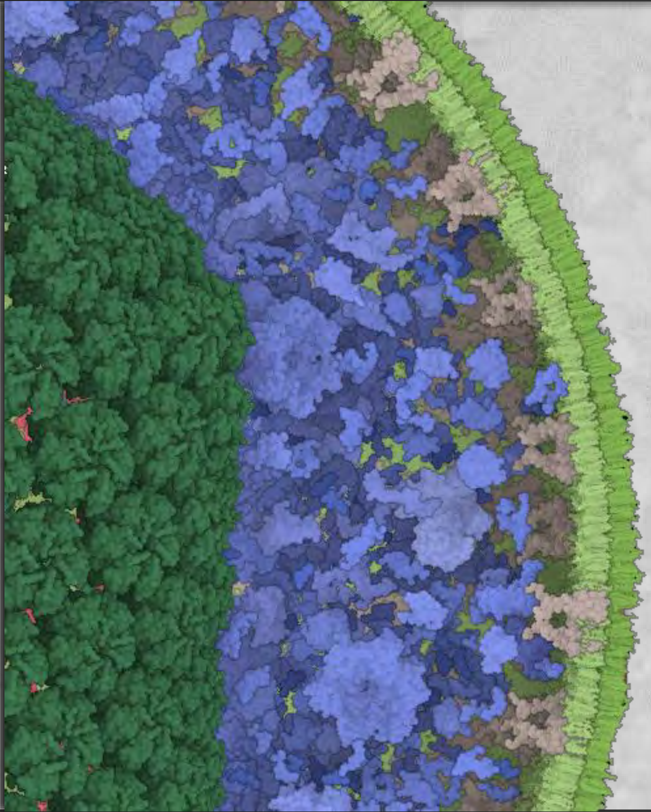
http://en.wikipedia.org/wiki/Protein_structure

Visualization Challenges

- Huge Models
- Multiple Scales
- Crowded Environment
- Multiple Instances
- Truly 3D Structures



Technology to Deliver



- Accurate Construction
- Interactive Rendering
- Multi-Scale Visualization
- Occlusion Management
- Guidance and Navigation
- Conveying Time

CONSTRUCTION

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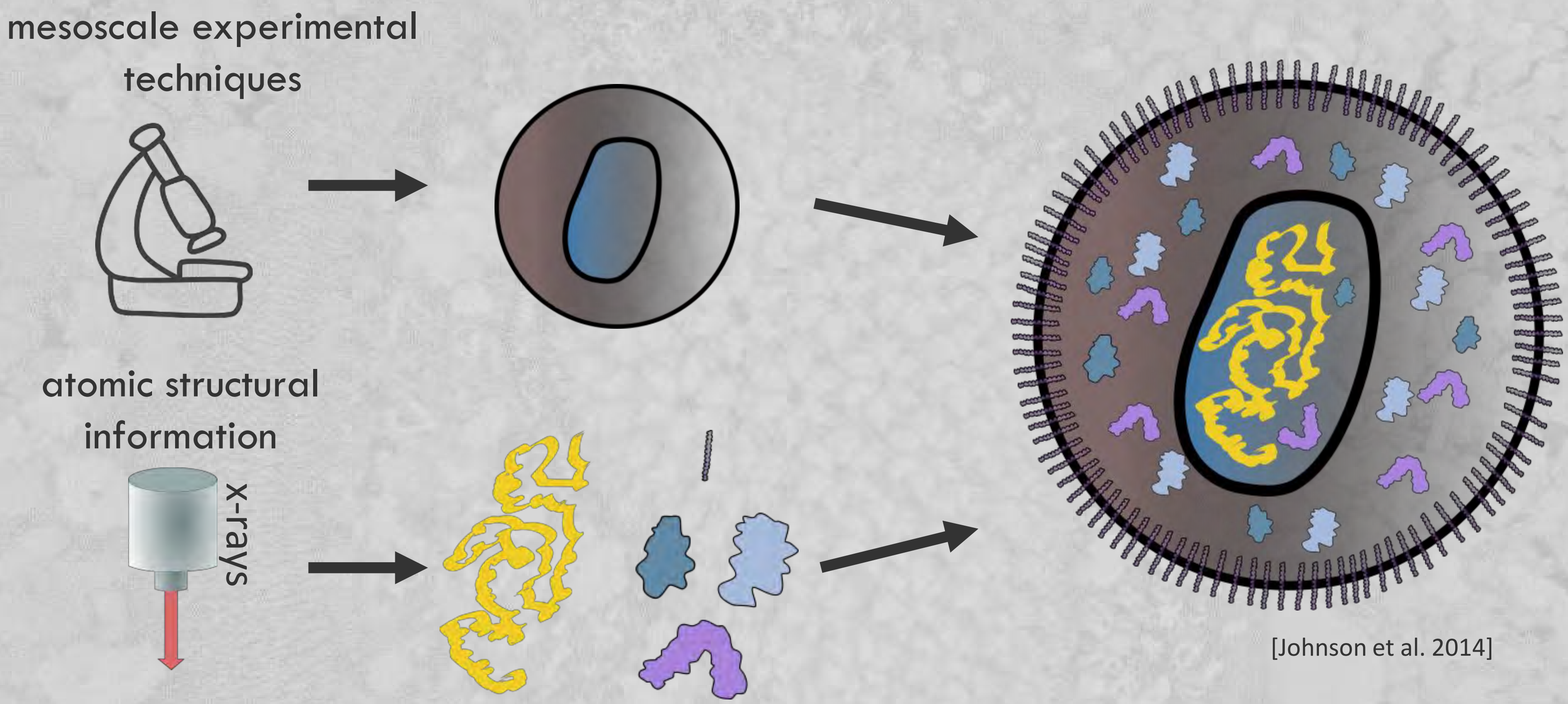
Integration of Molecular and Cell Biology



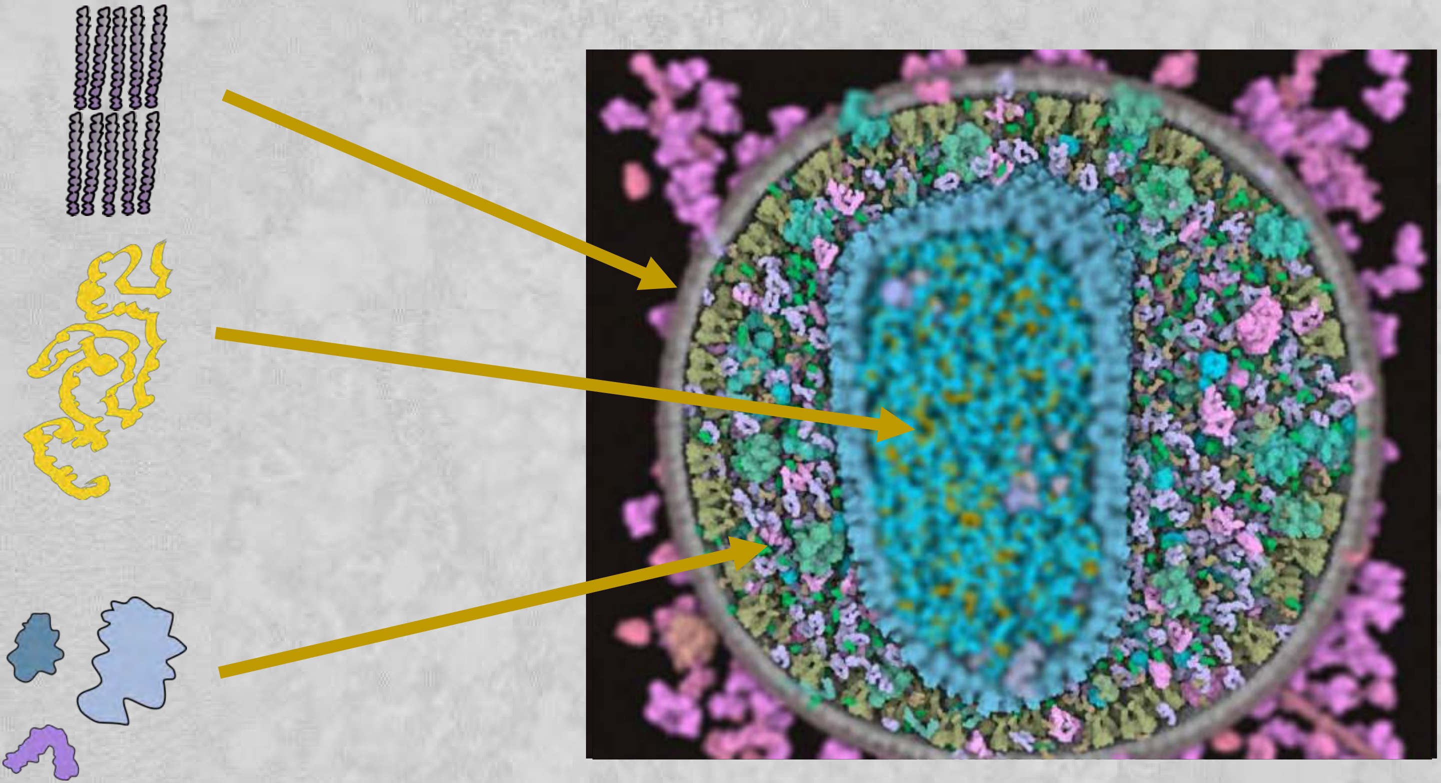
[Johnson et al. 2014]

Ingredients

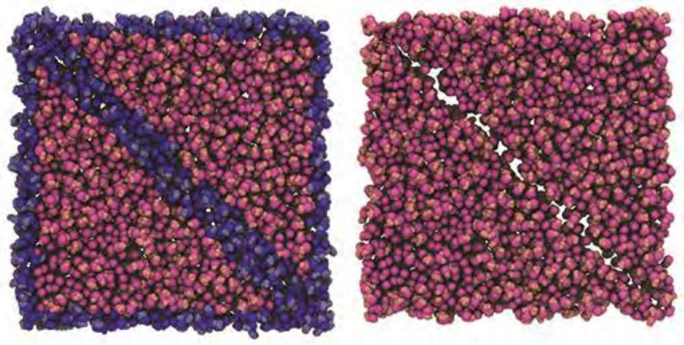
membrane

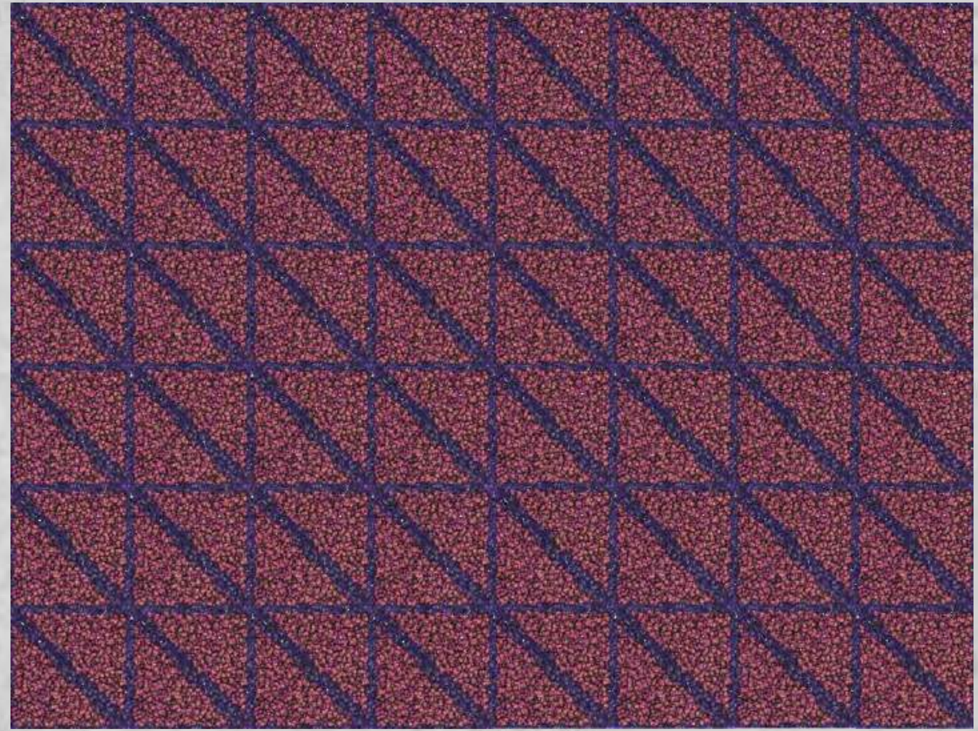
fibrous structures

solubles



Memory-Hungry Lipid Generation

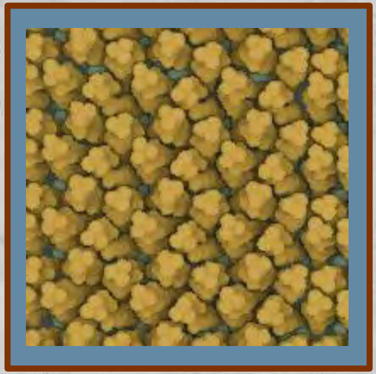


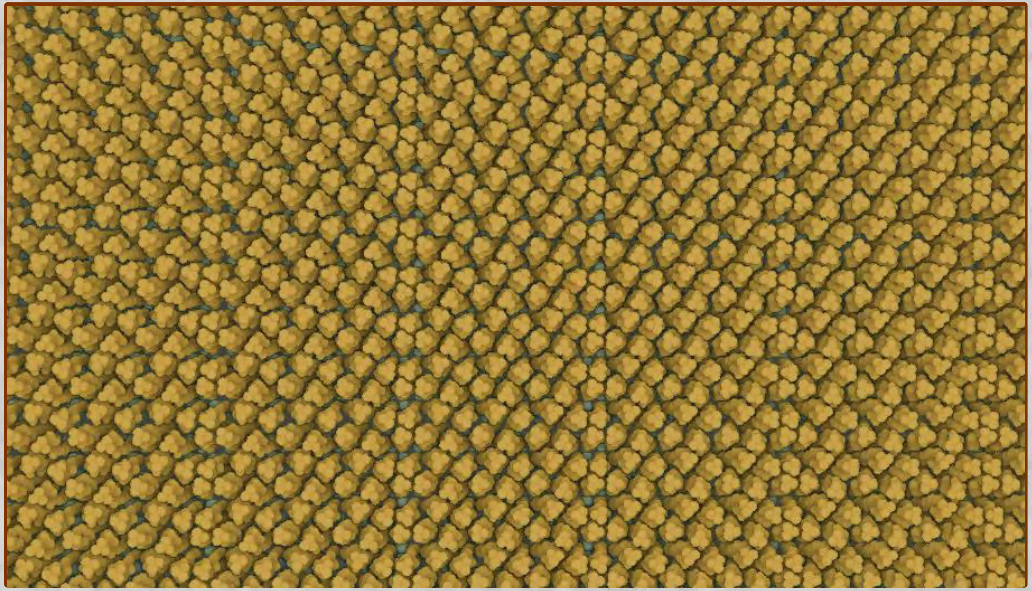


[Durrant and Amaro 2014]

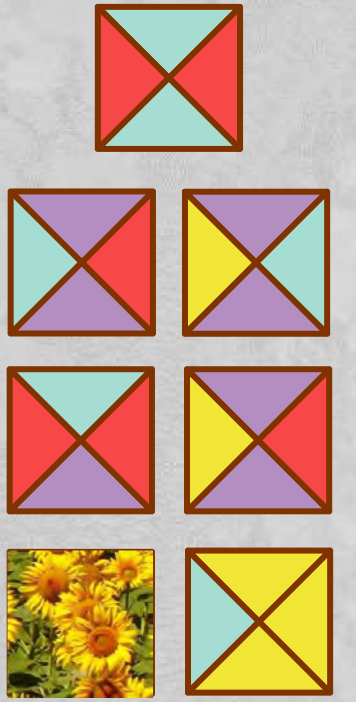
Periodic Membrane Population

texture tile





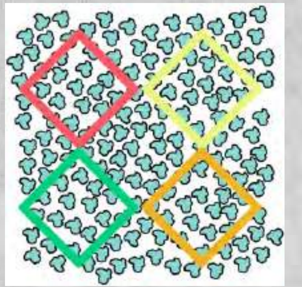
Memory Efficient Aperiodic Tiling



[Wang 1961]

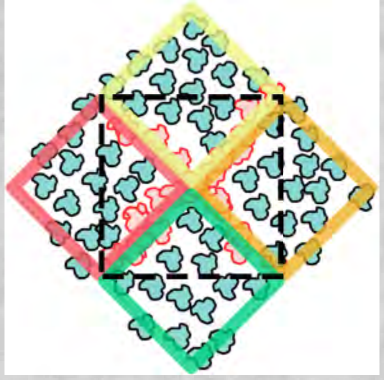
Membrane Population Algorithm

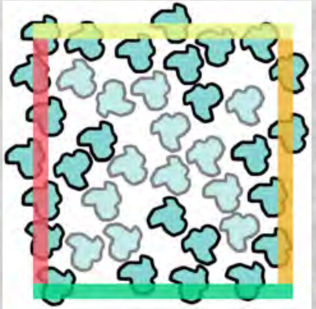
1. Choose patches



3. Remove overlaps

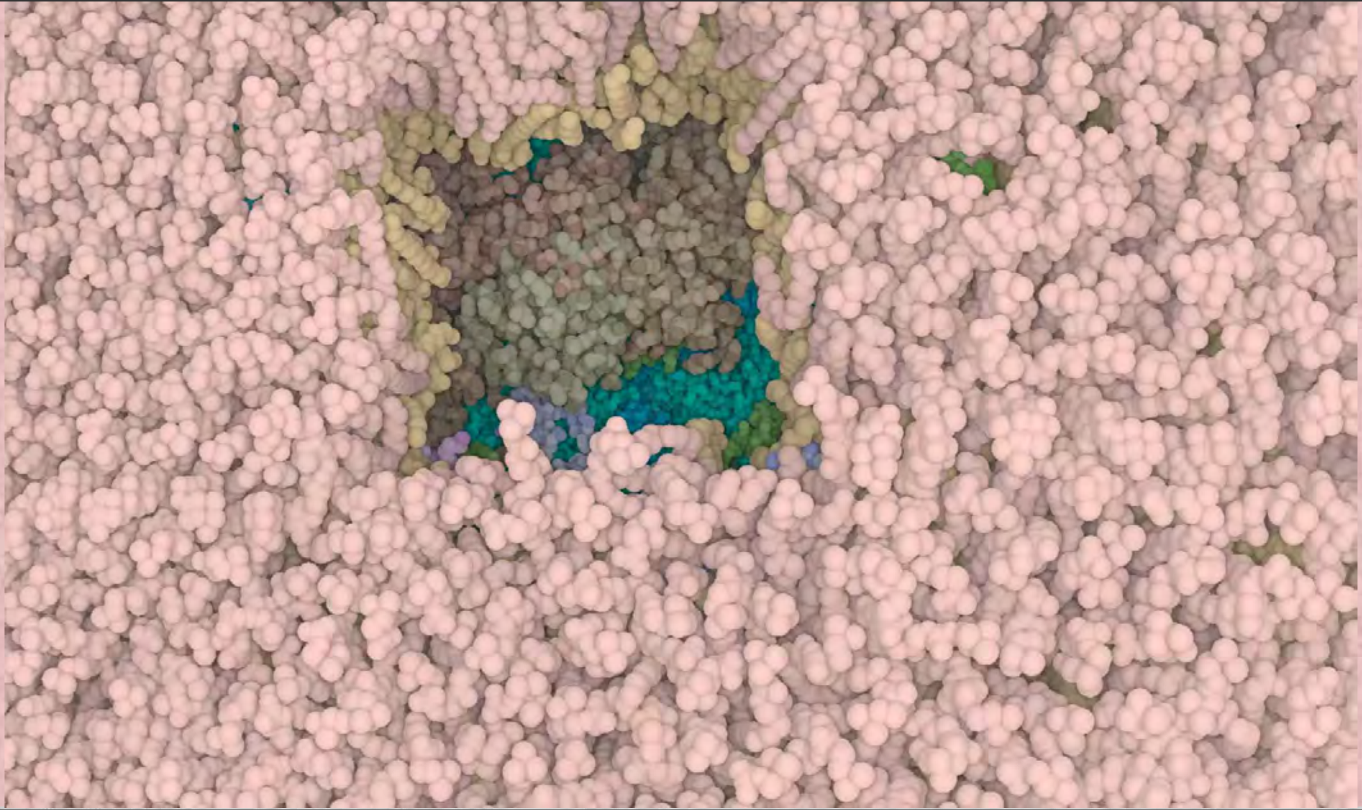
2. Combine to tile





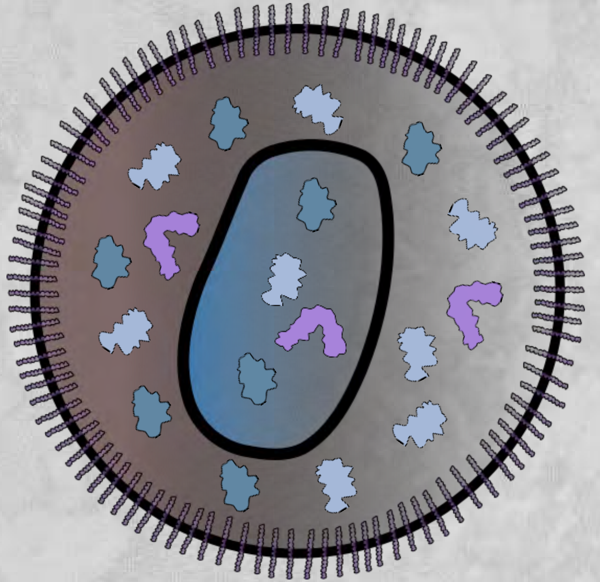
4. Fill gaps

Membrane Population Algorithm

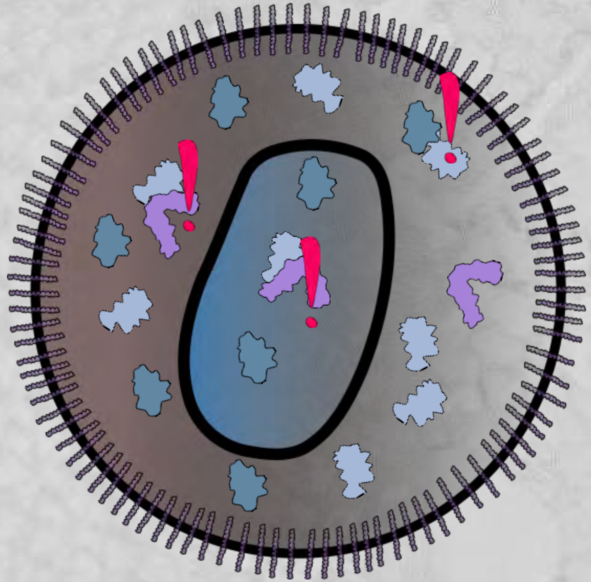


Soluble Population Algorithm

Previous approach
- Iterative population



Our approach
- 3-step parallel population



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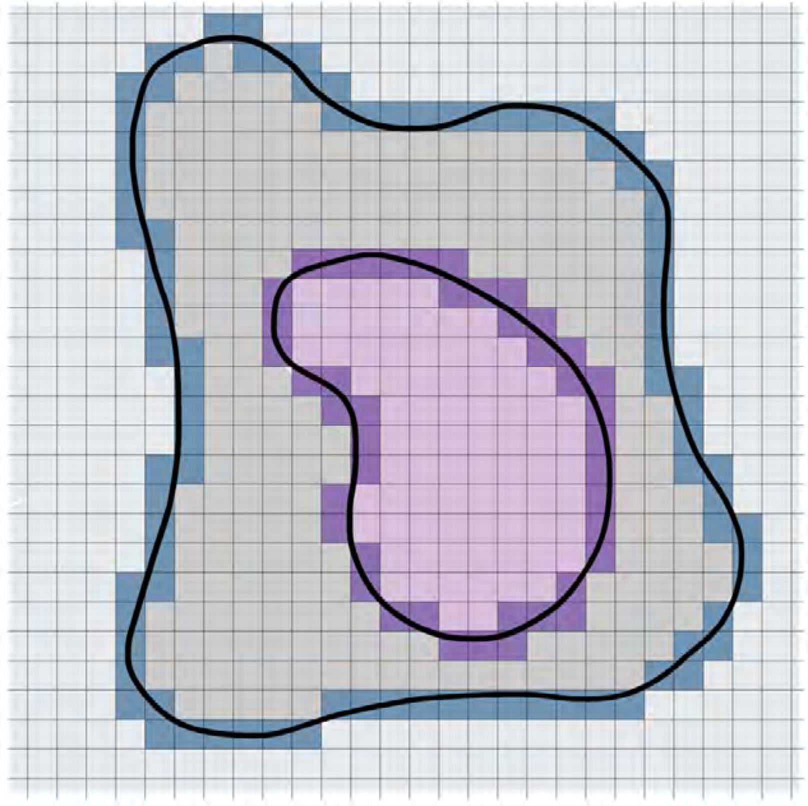
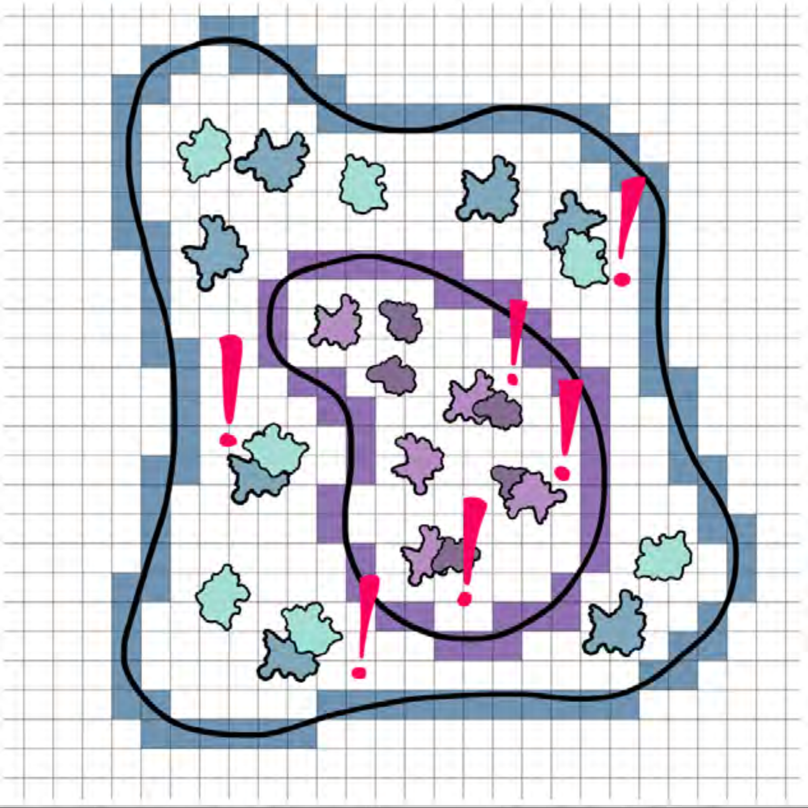
Soluble Population Algorithm

1. Compartment and occupancy grid



Soluble Population Algorithm

1. Compartment and occupancy grid
2. Populate molecules into compartments



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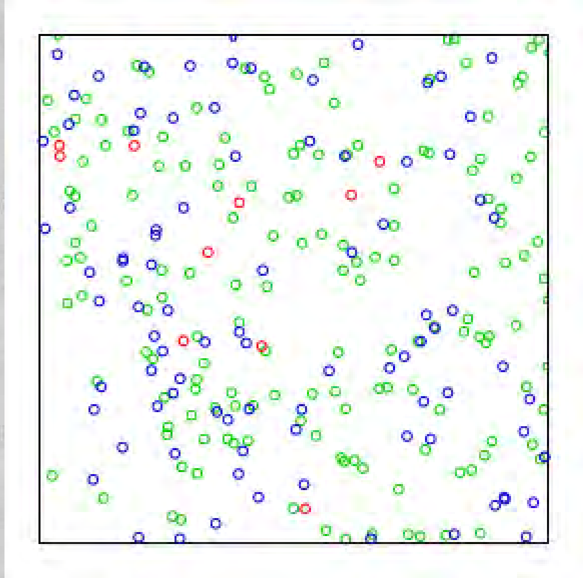
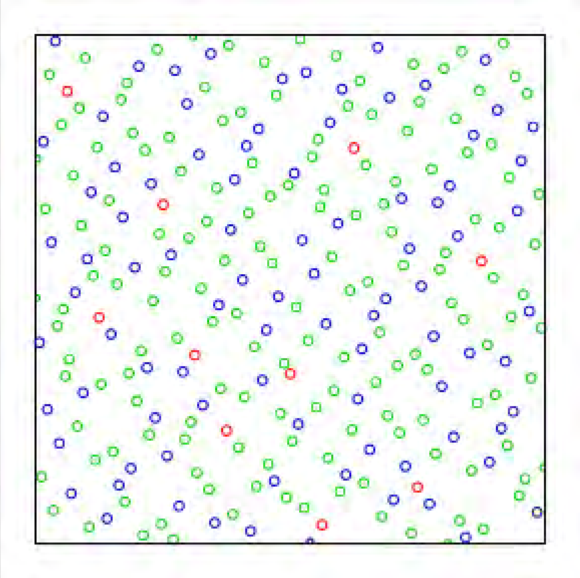
Evenly-Spaced Distribution

pseudorandom number



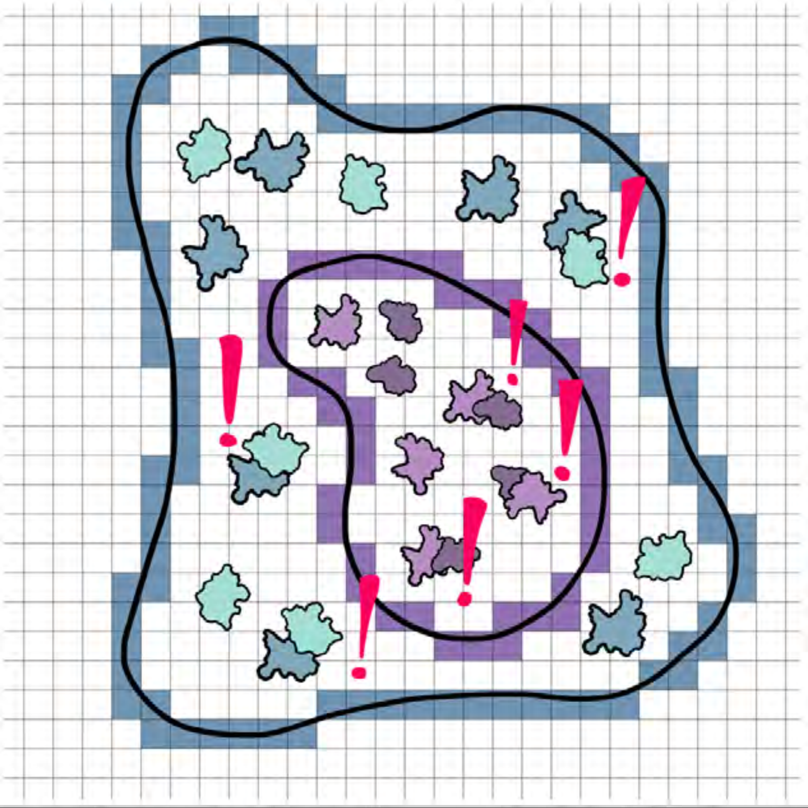
Halton sequence



[Willmott 2007]

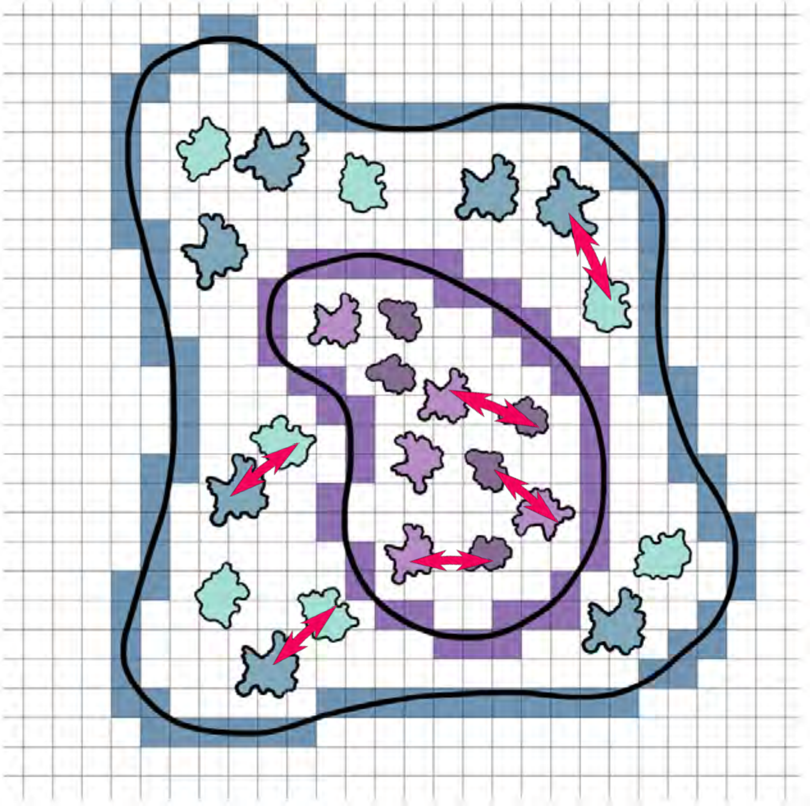
Soluble Population Algorithm

1. Compartment and occupancy grid
2. Populate molecules into compartments



Soluble Population Algorithm

1. Compartment and occupancy grid
2. Populate molecules into compartments
3. Resolve overlaps and update ccupancy grid



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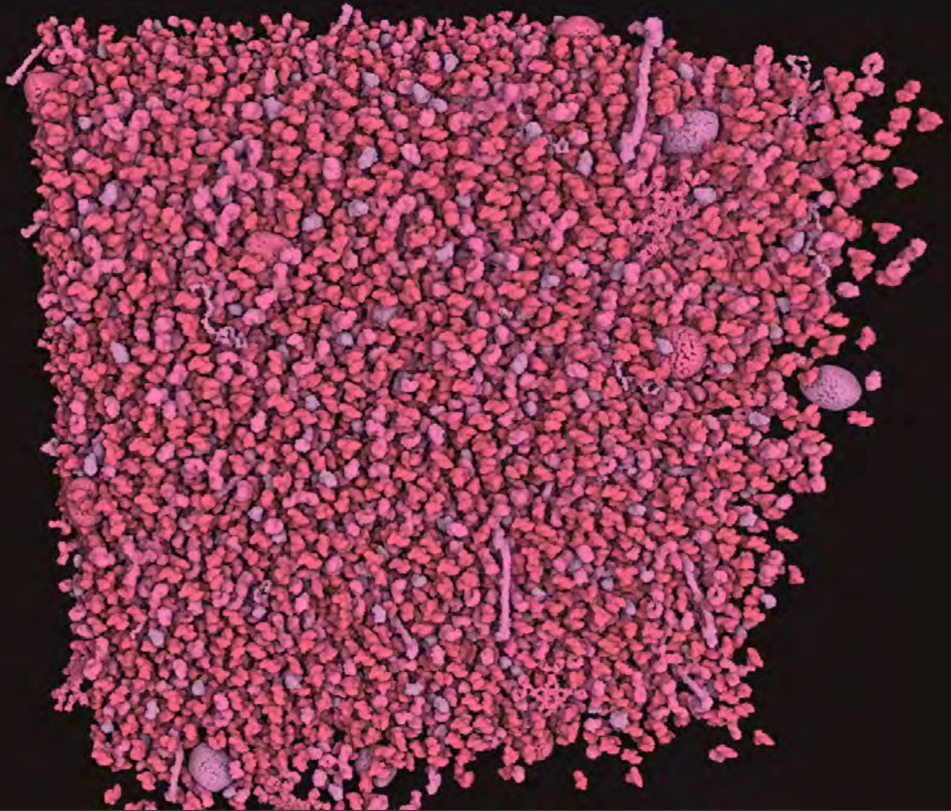
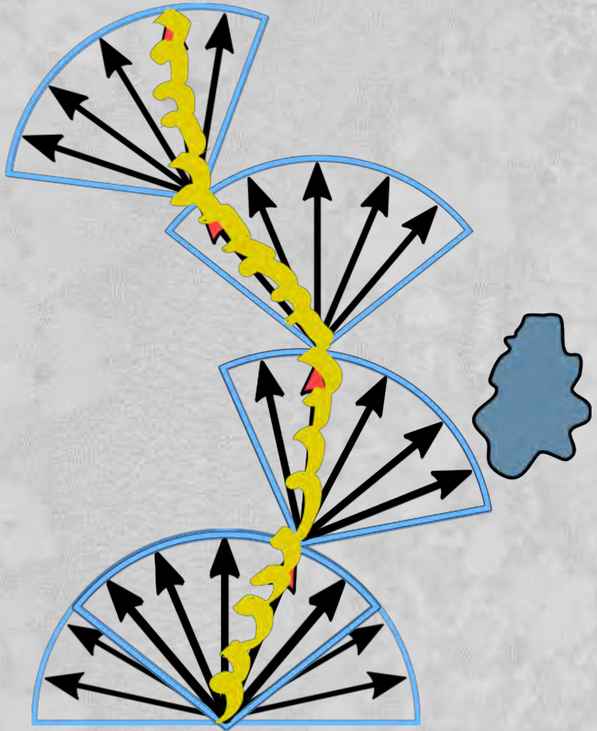
Soluble Population Algorithm



Fiber Growing Algorithm



short persistance length

long persistance length

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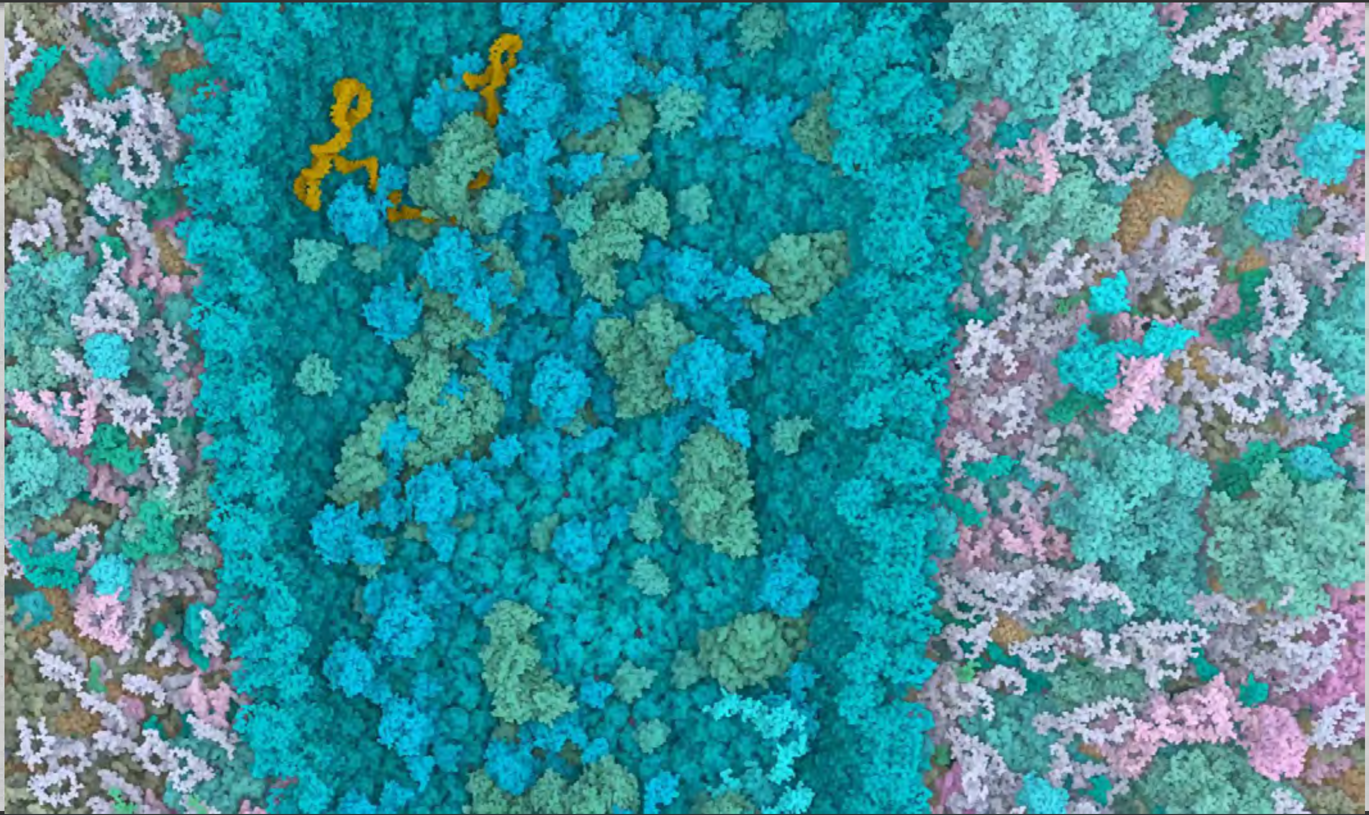
Fiber Growing Algorithm



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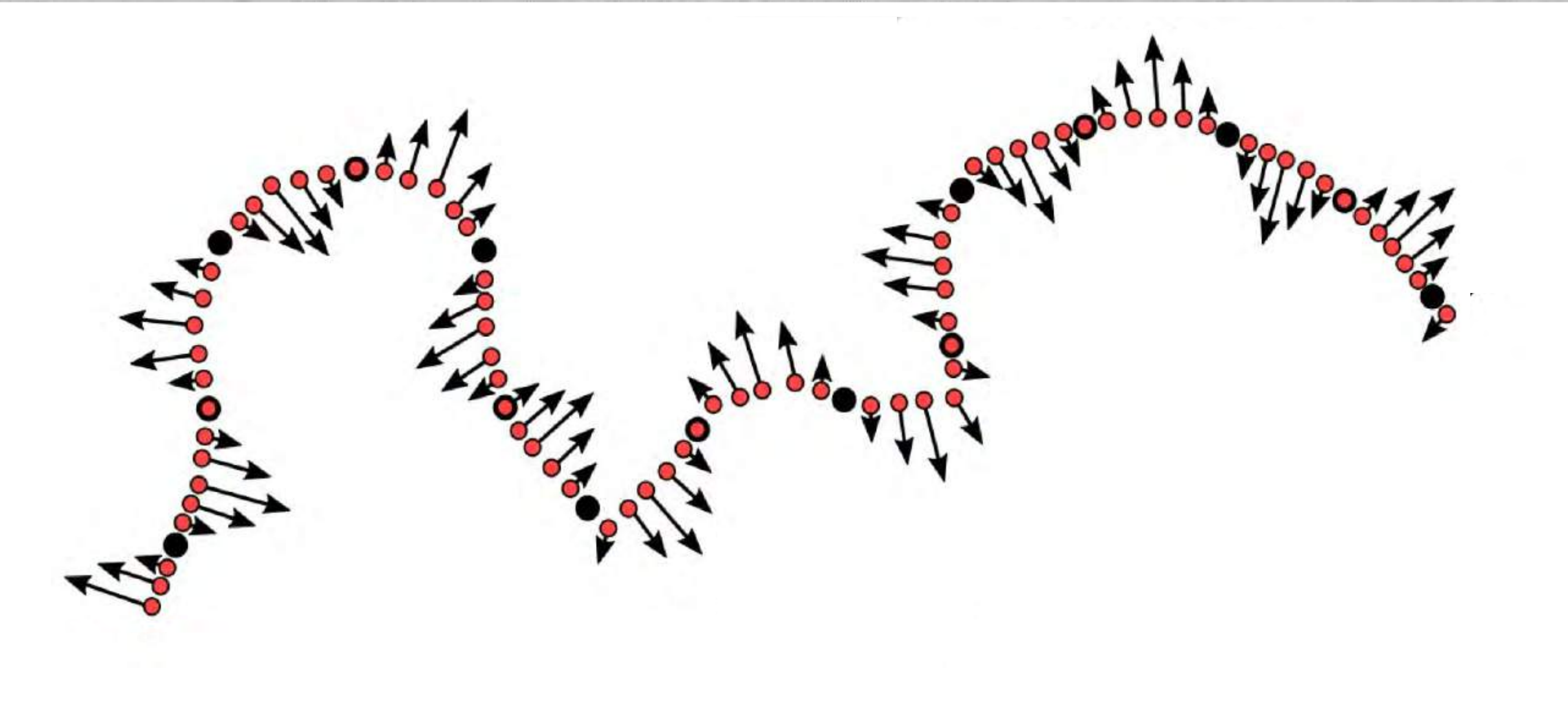
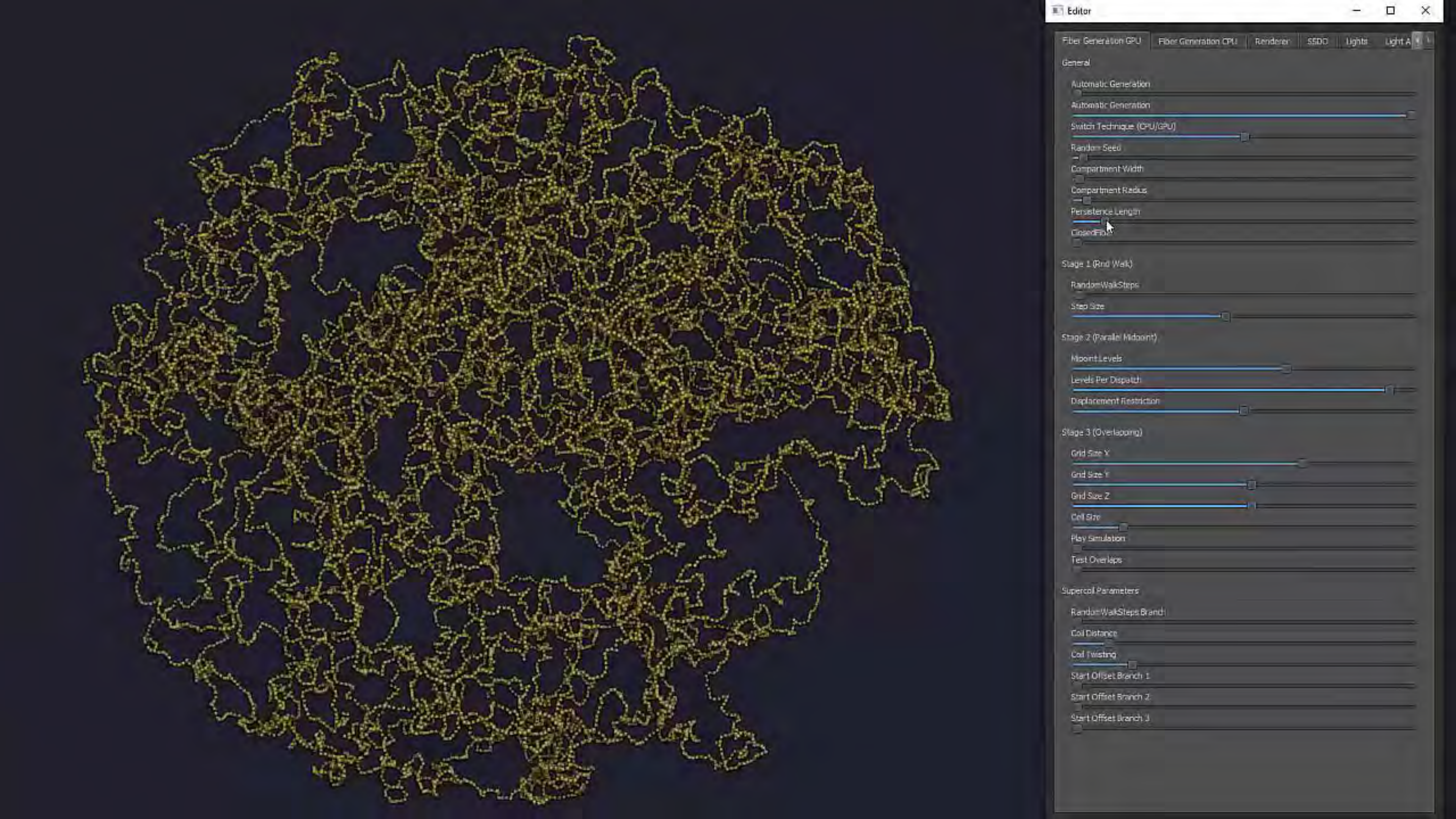
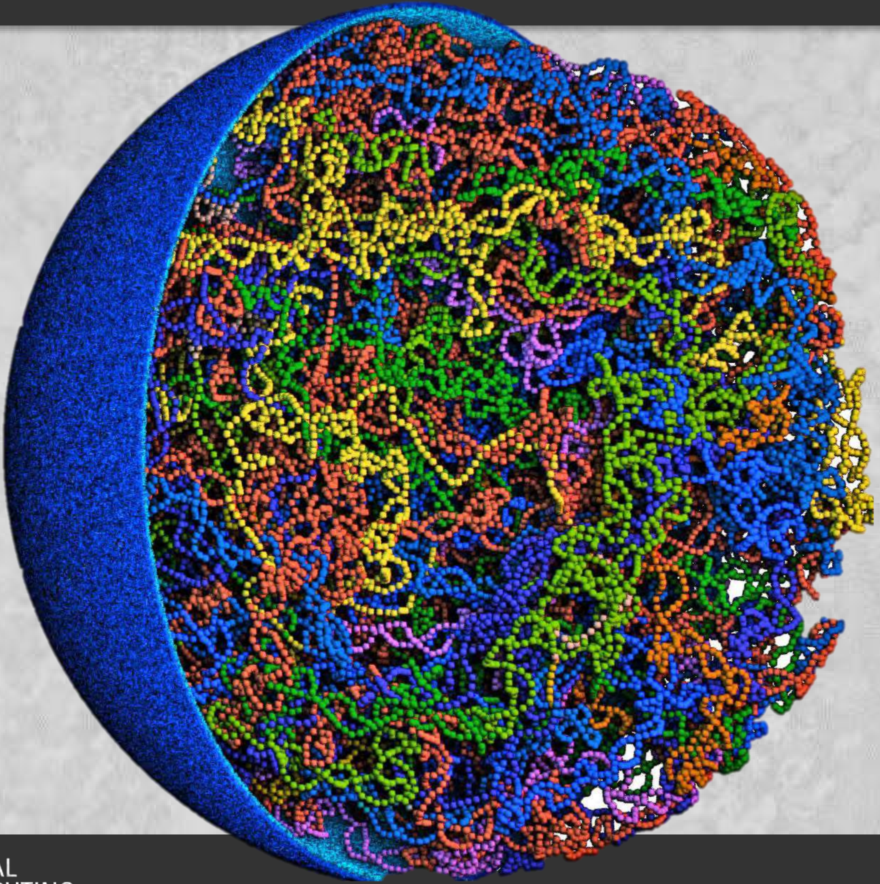
Parallel Fiber Construction Algorithm




Editor
Fiber Generation GPU
Fiber Generation CPU
Renderer
SSDO
Lights
General
Automatic Generation
Automatic Generation
Switch Technique (CPU/GPU)
Random Seed
Compartment Width
Compartment Radius
Persistence Length
Stage 1 (Rnd Walk)
RandomWalkSteps
Step Size
Stage 2 (Parallel Midpoint)
Midpoint Levels
Levels Per Dispatch
Displacement Restriction
Stage 3 (Overlapping)
Grid Size X
Grid Size Y
Grid Size Z
Cell Size
Play Simulation
Test Overlaps
Supercoil Parameters
RandomWalkSteps Branch
Coil Distance
Coil Twisting
Start Offset Branch 1
Start Offset Branch 2
Start Offset Branch 3

Mycoplasma DN



RENDERING

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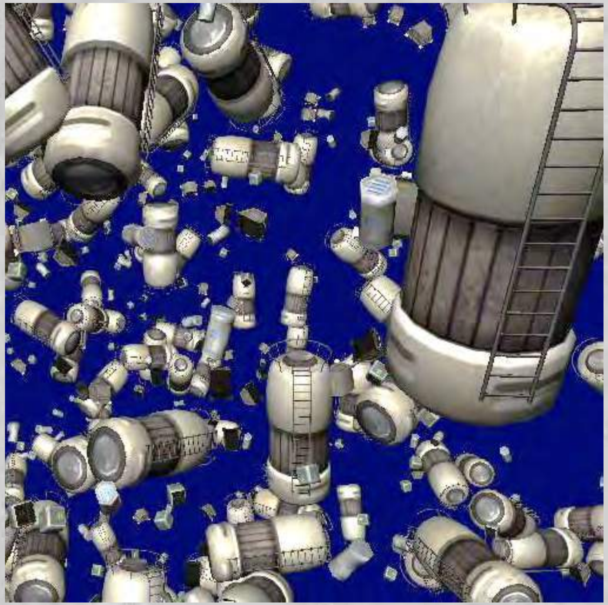
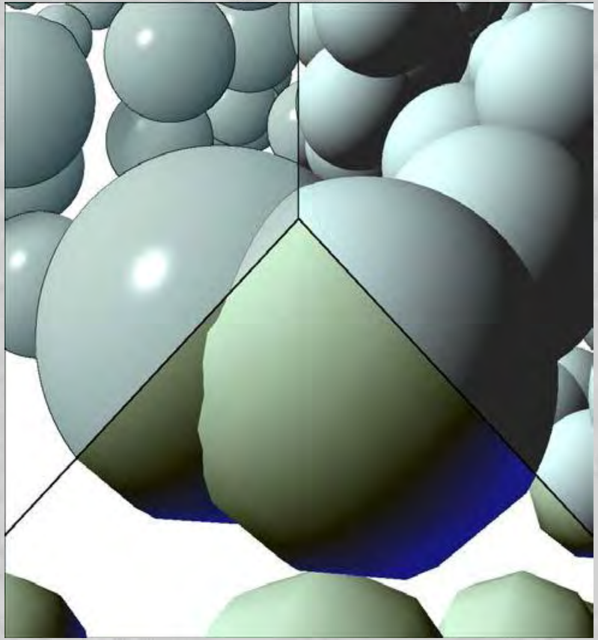
Instancing

- Draw procedures render one object per draw call
- Identical objects (trees, plants, …)
  can be rendered in a *for* loop
- Instancing allows to render one object
  multiple times in single draw call
- This results in significant speedup
  as compared to thousands of draw calls
- Store all information on the GPU
- Position / rotation differ for each instance



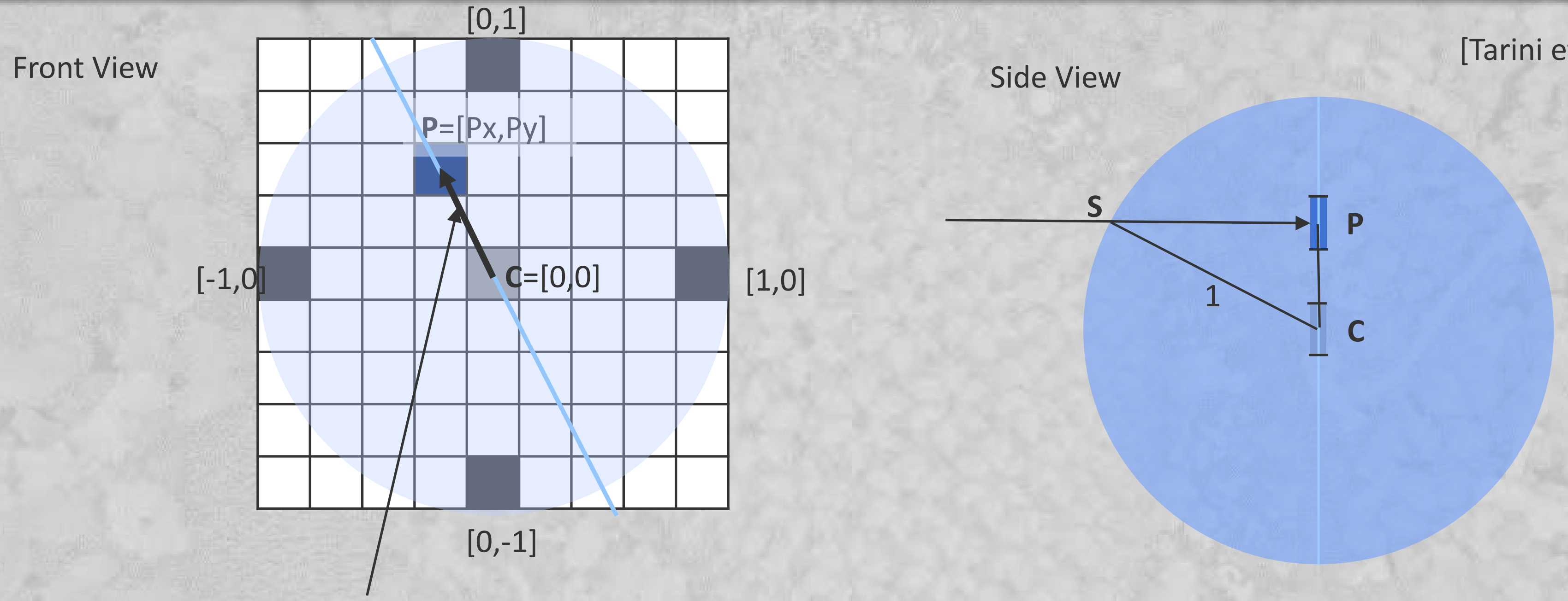
Procedural Impostors for Atom Rendering

- Impostors
  - have baked-in shading
  - are planar in depth
- Procedural Impostors
  - have pixel precise quality
  - have correct depth
  - lighting is calculated on the fly



Procedural Impostors

[Tarini et al. 2006]



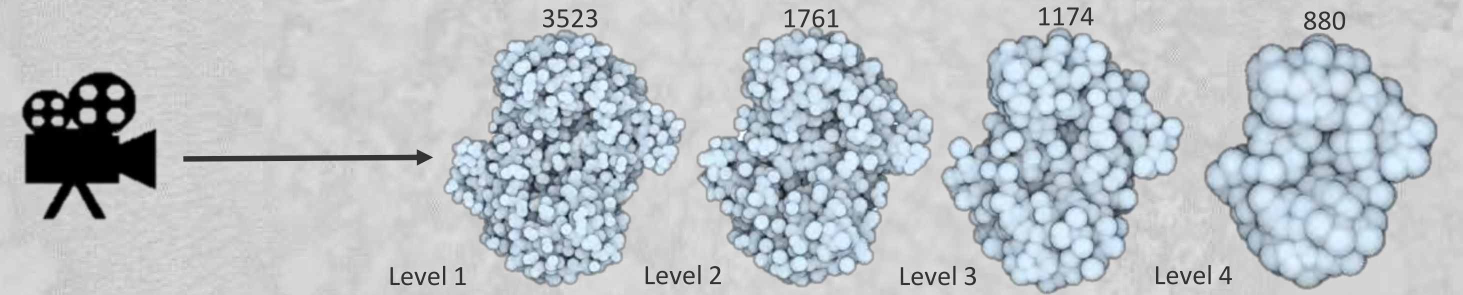
CP = [Px-Cx,Py-Cy]

|**CP**| = sin(∠SCP) ➔ |**SP**| = $(1 - |\mathbf{CP}|^2)^{1/2}$

CS = **CP** + **PS**

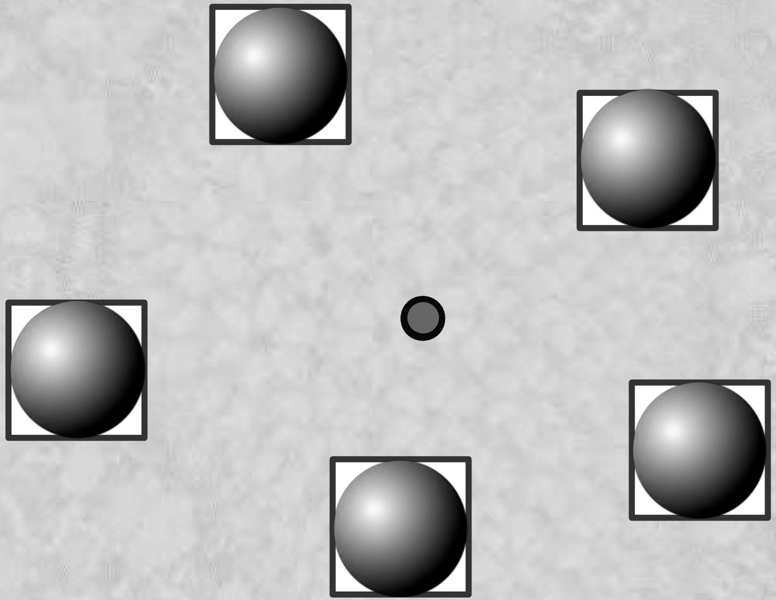
Heuristic Level-of-Detail Representation

- Sort atoms based on distance from center
- With increasing distance from the molecule
  - Skip every k atoms while preserving shape
  - Increases atom size with distance



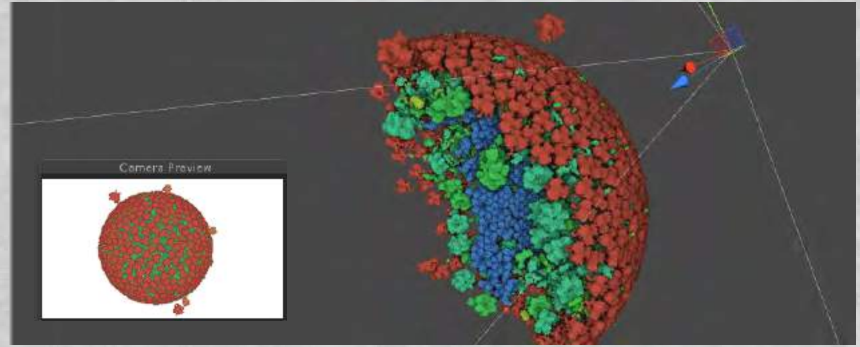
Mathieu Le Muzic, Ivan Viola

View-Guided Emitting of Geometry



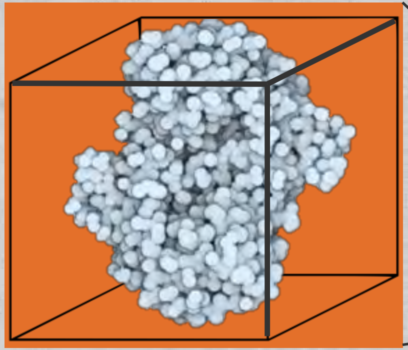
Occlusion Culling with Hierarchical Z-Buffer

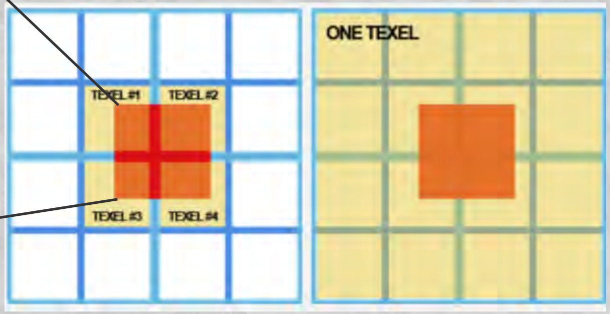
- Render molecules from previous frame
- Z-Buffer and Mip-Map levels are created
- Hierarchical Z-Buffer and molecule BB tests for visibility of previously invisible molecules



[Greene et al. 1993]
[Le Muzic et al. 2015]

Hierarchical Z-Buffer





http://rastergrid.com/blog/2010/10/hierarchical-z-map-based-occlusion-culling/

VISUALIZATION

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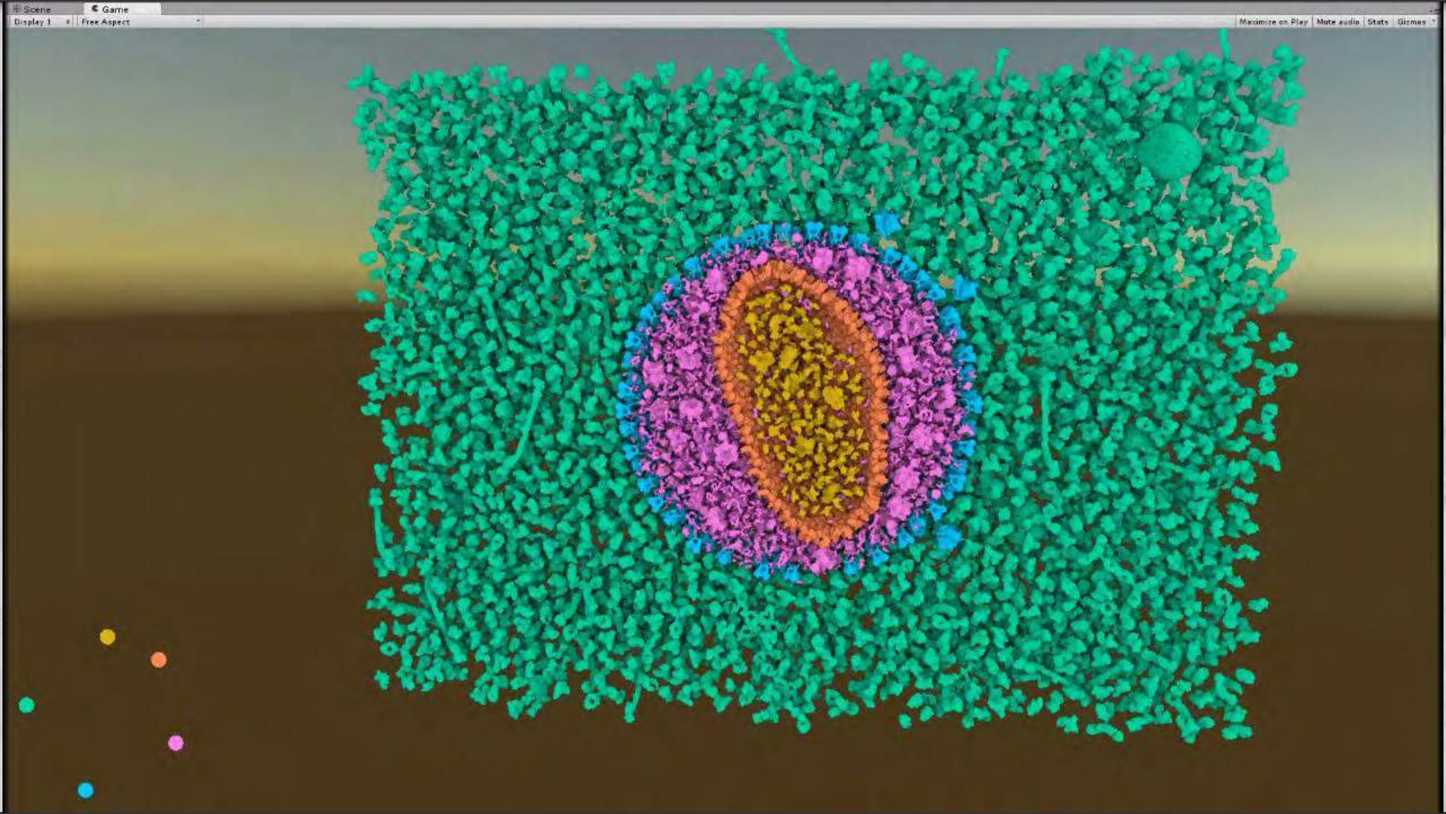
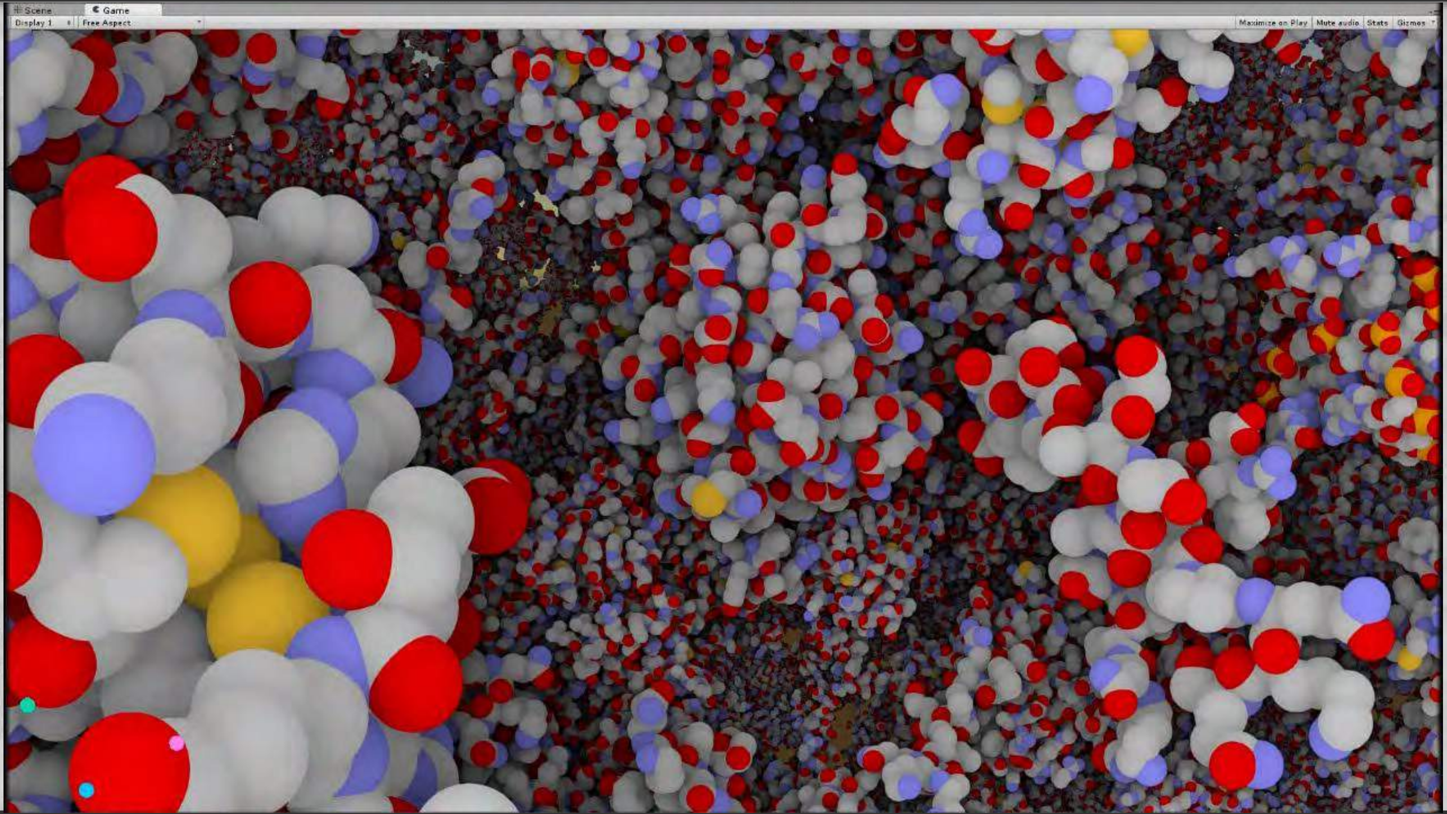
Multi-Scale Illumination

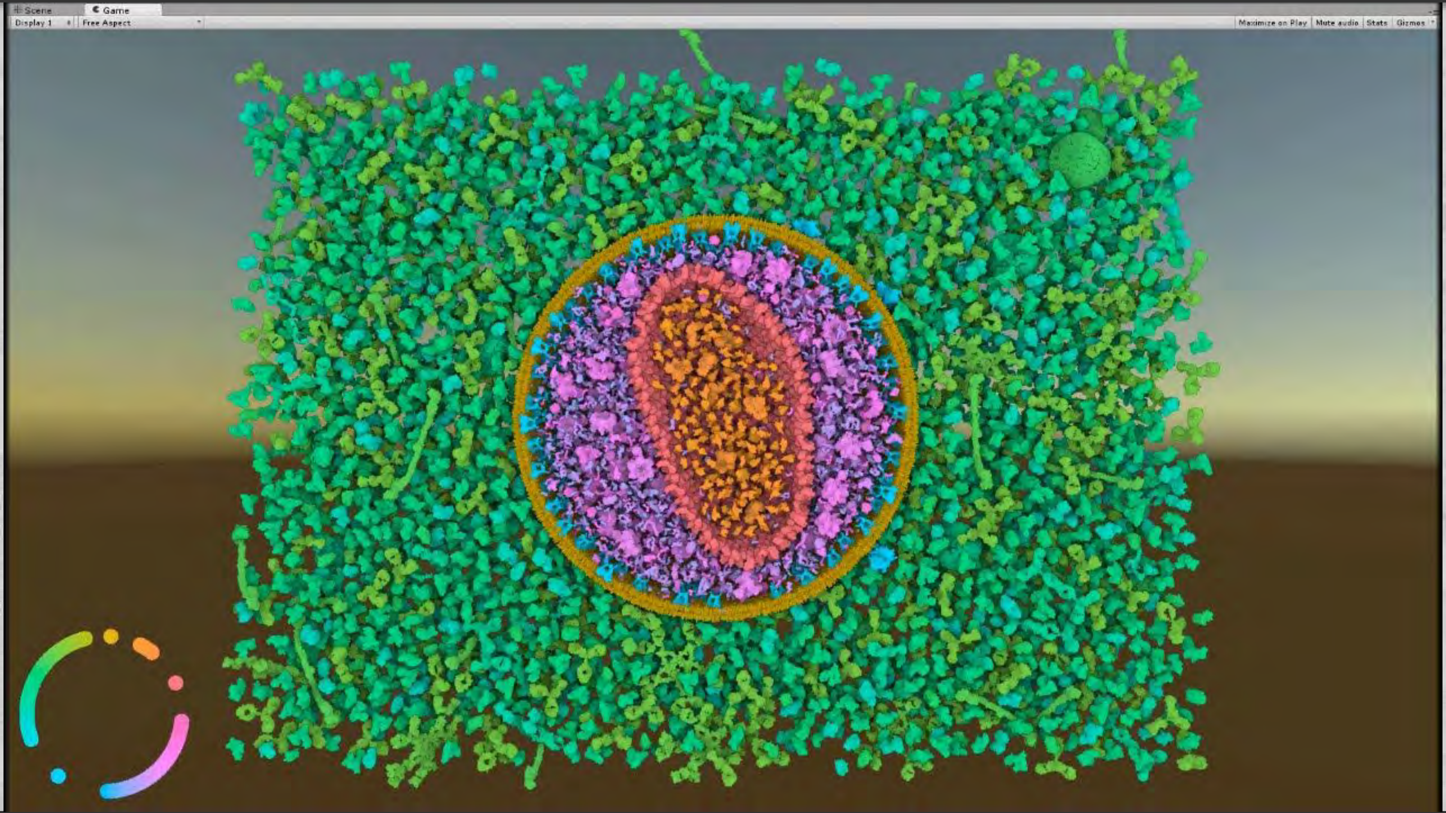
Multi-Scale Coloring Problem



Multi-Scale Coloring Problem



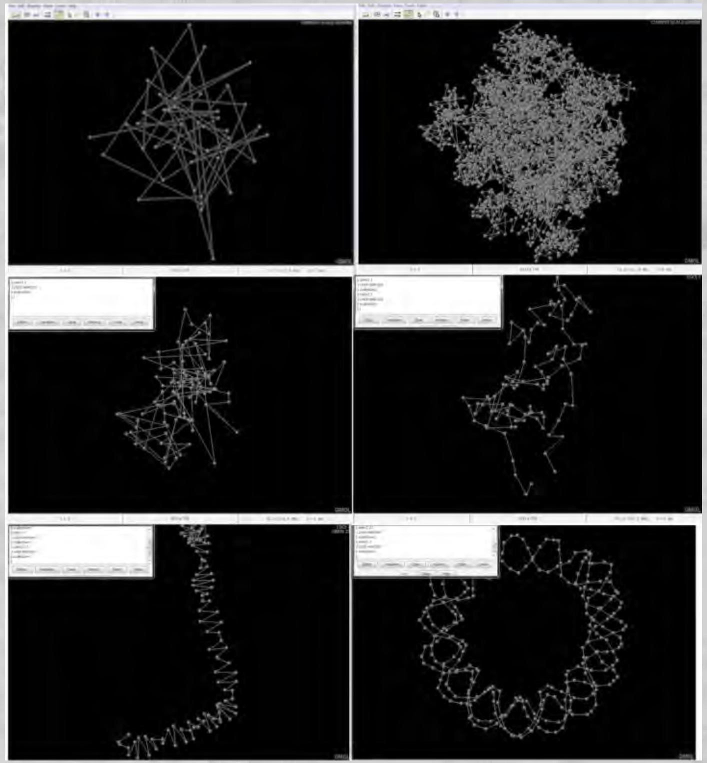
Multi-Scale Coloring Algorithm



Nicholas Waldin, Ivan Viola

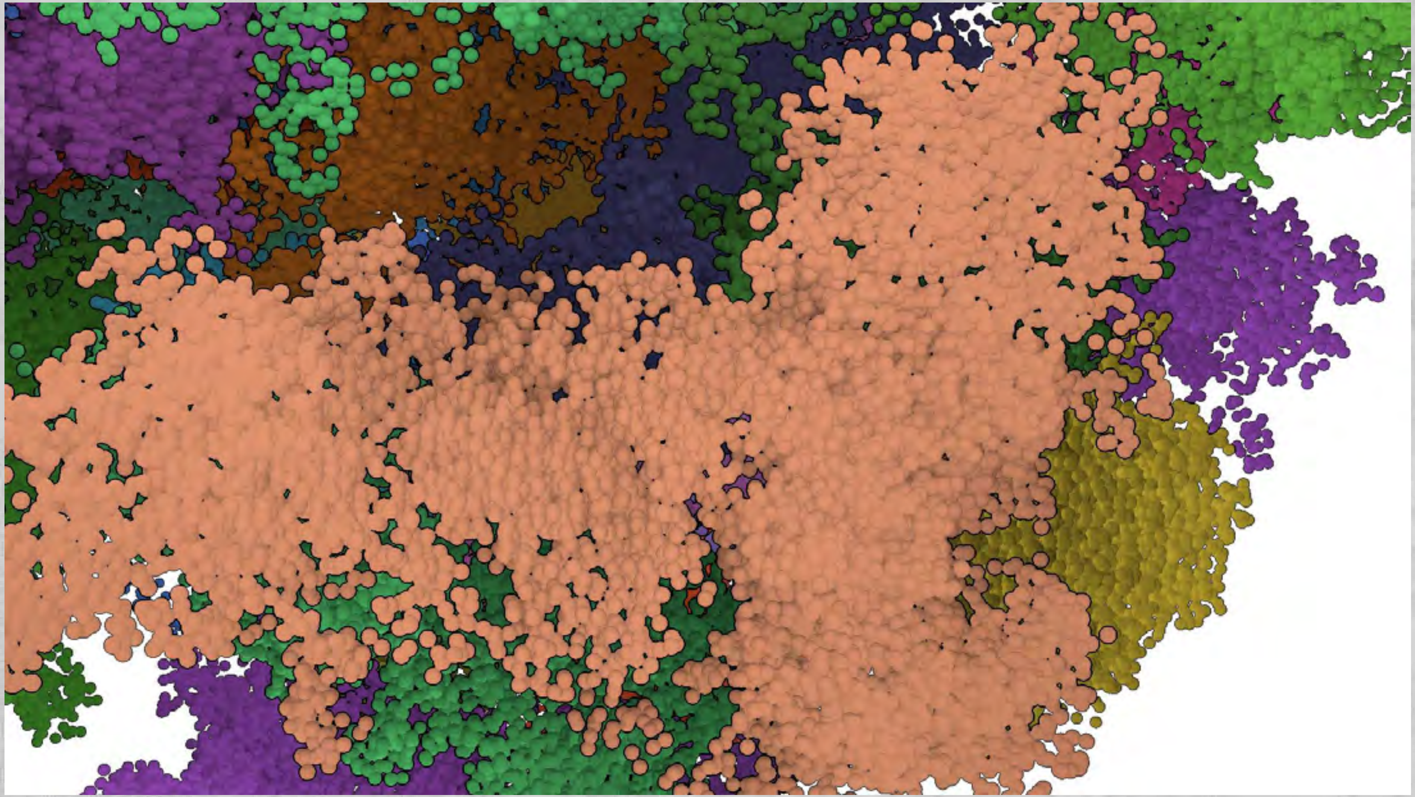
Human Interphase DNA Visualization

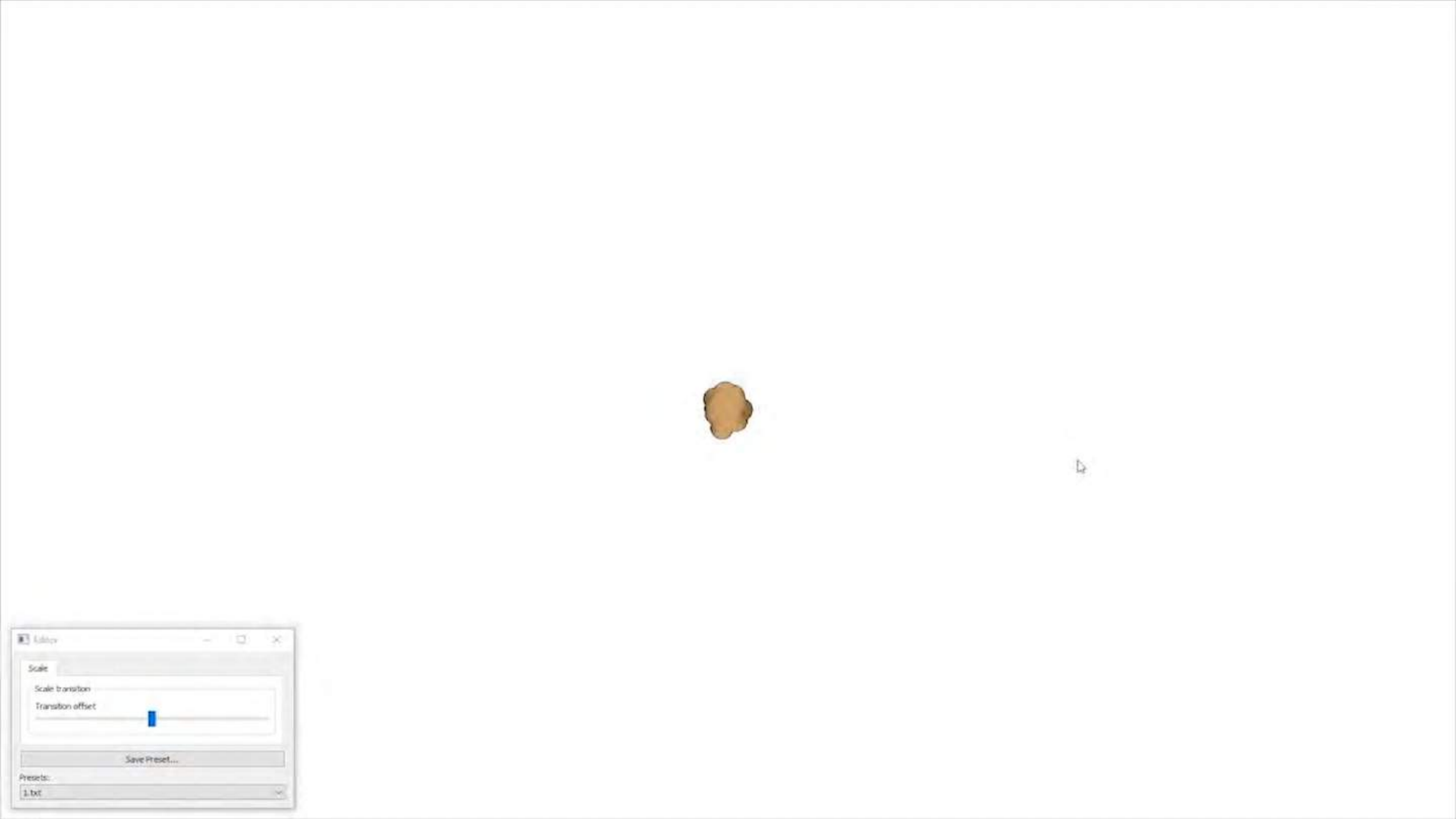
- Dataset containing points for various scales
- Nucleosomes, fiber, loci, chromosome
- Can we traverse it with a realistic structural depiction?



[Novotny et al., 2016]

Human Interphase DNA Visualization




Editor
Scale
Scale transition
Transition offset
Save Preset...
Presets:
1.txt

DNA-NANOTECHNOLOGY VISUALIZATION

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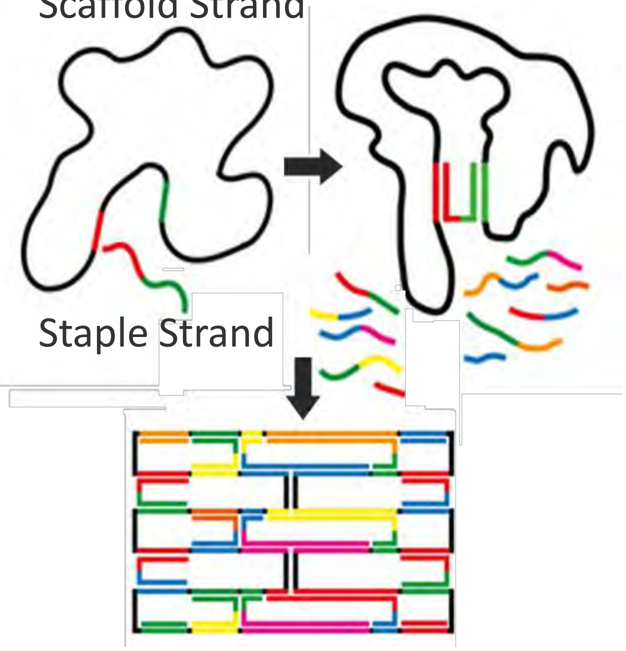
DNA Nanotechnology | Self-Assembly



Modified from openwetware.org

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GCCCTGGGGTCTCCTCGGGAACGGCAGTGAG
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ACTTTACCAGCAGAGCCCCAGTATAATCATAT
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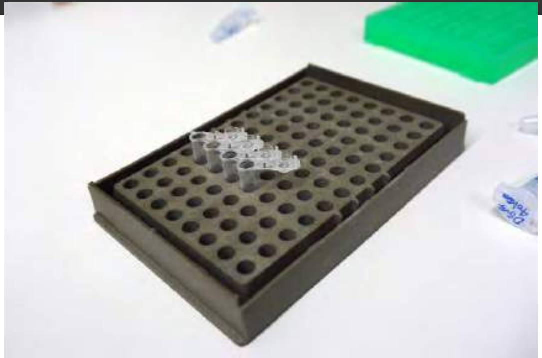
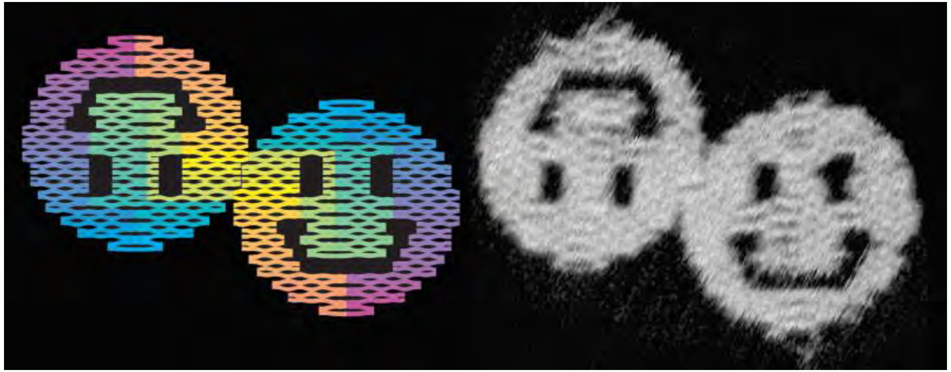


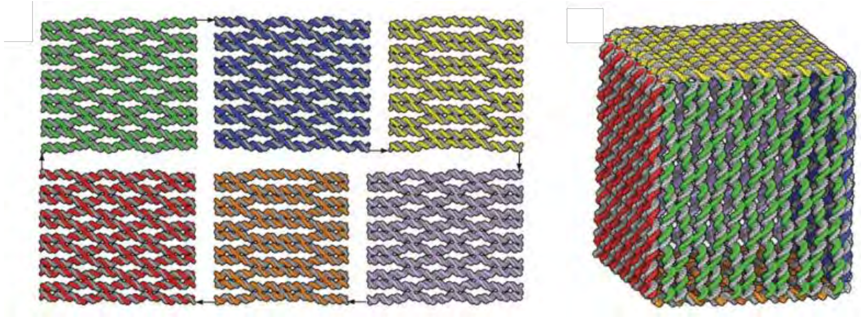
In Silico Design → DNA Sequence Export → Self-Assembly in the Lab

Haichao Miao, Ivan Viola

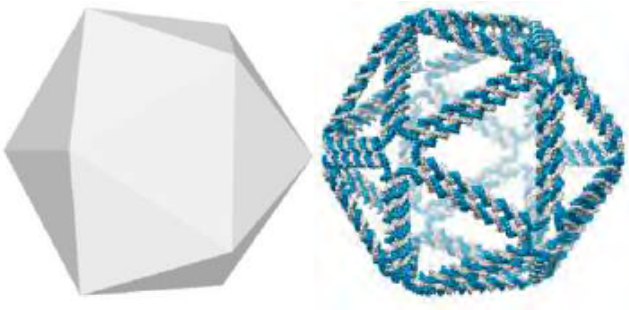
DNA Nanostructures



Rothemund 2006

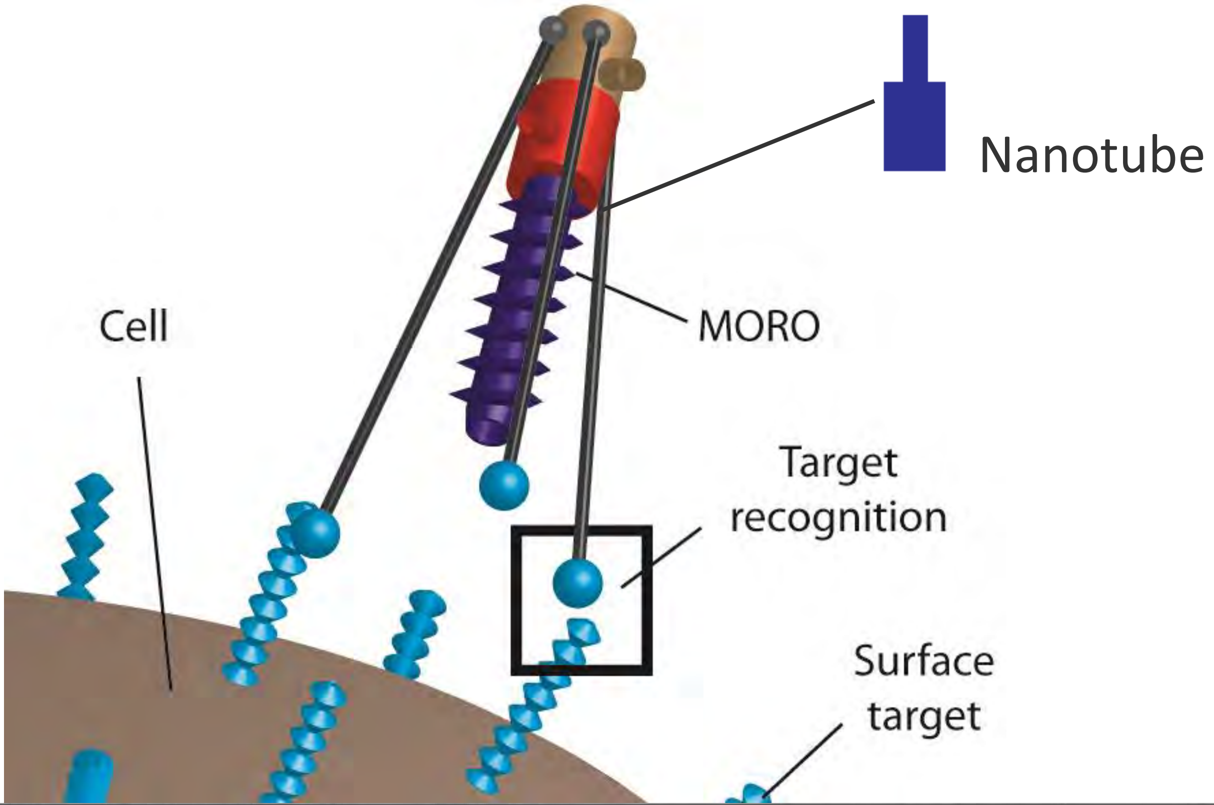


Andersen et al. 2009

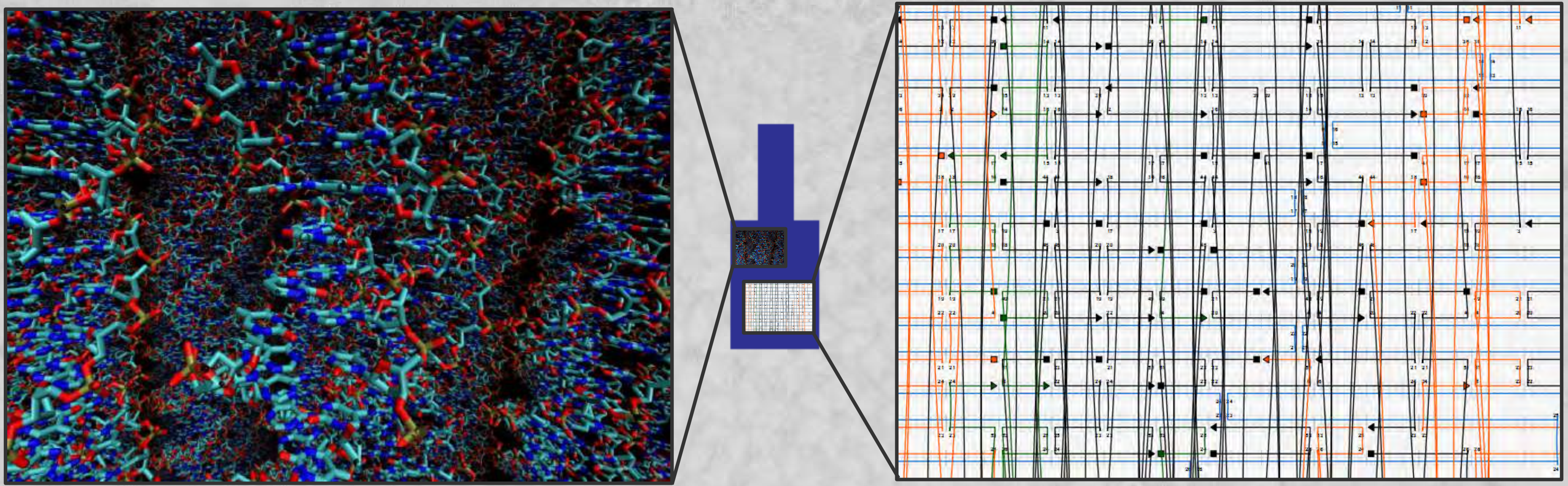


Veneziano et al. 2016

Final Project Goal: DNA Nanorobot



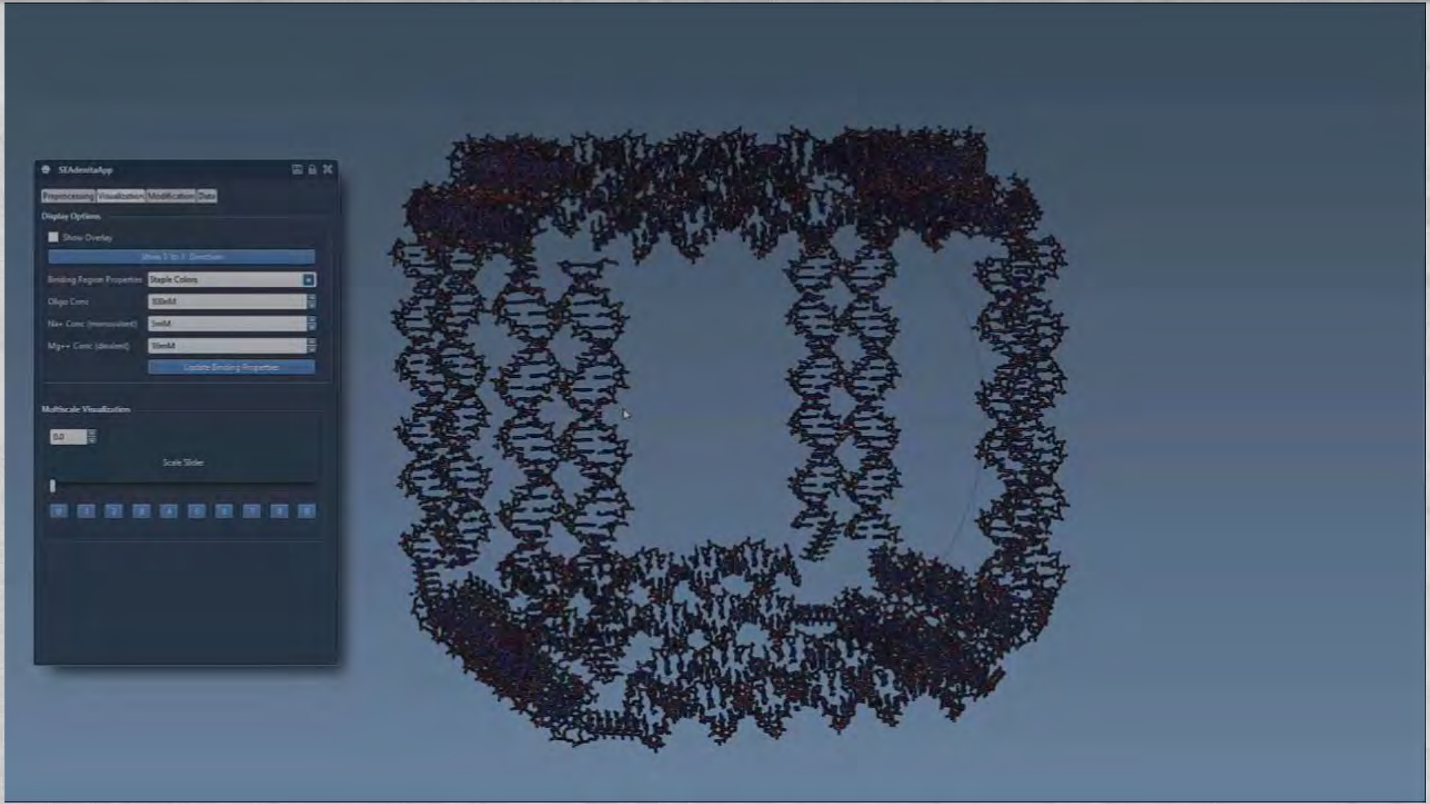
Motivation | Nanotube



Low-Level
All-Atoms

High-Level
Schematics

Seamless Transition Across Scales



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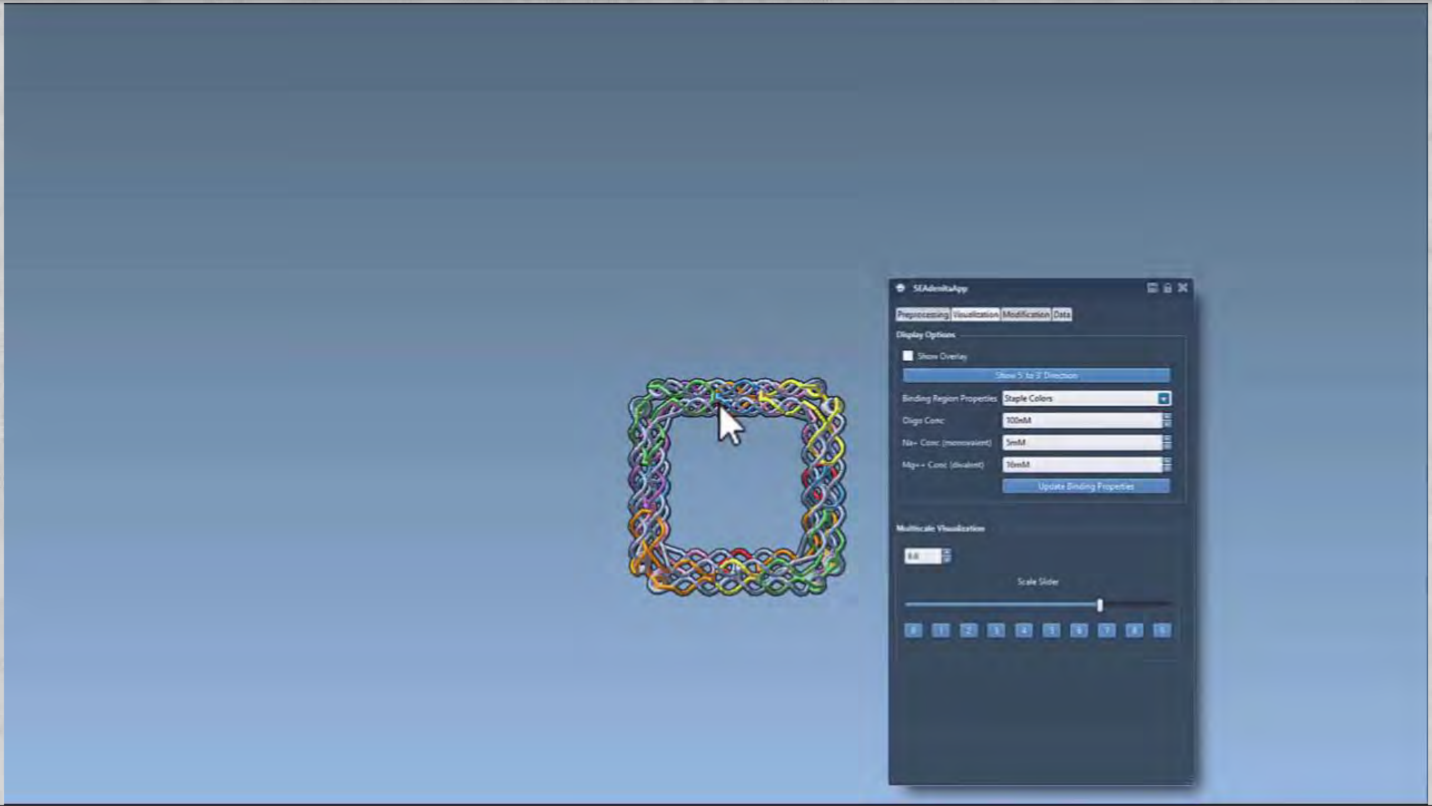
Scale-Adaptive Modifications | Break & Concatenate



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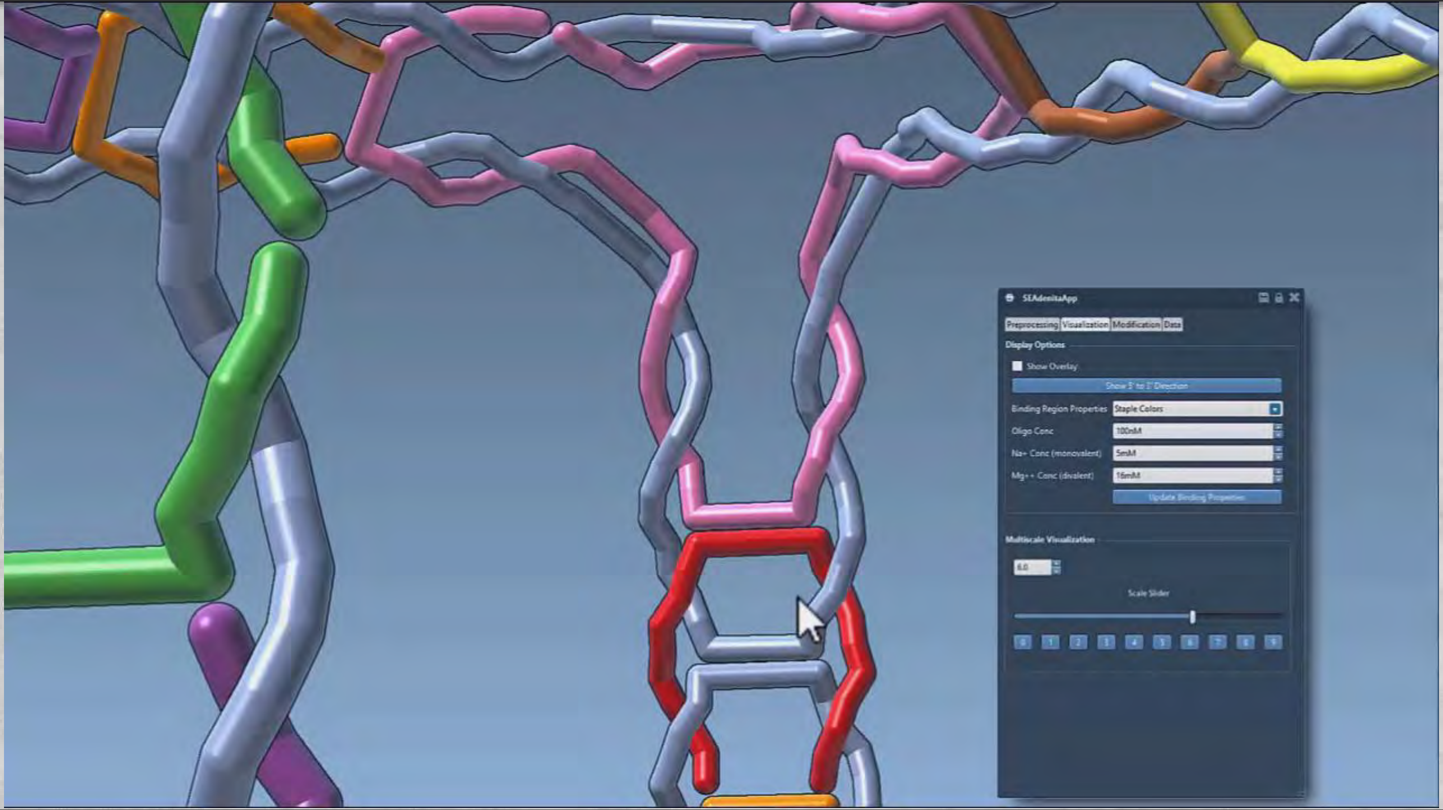
Task: Strand Merging



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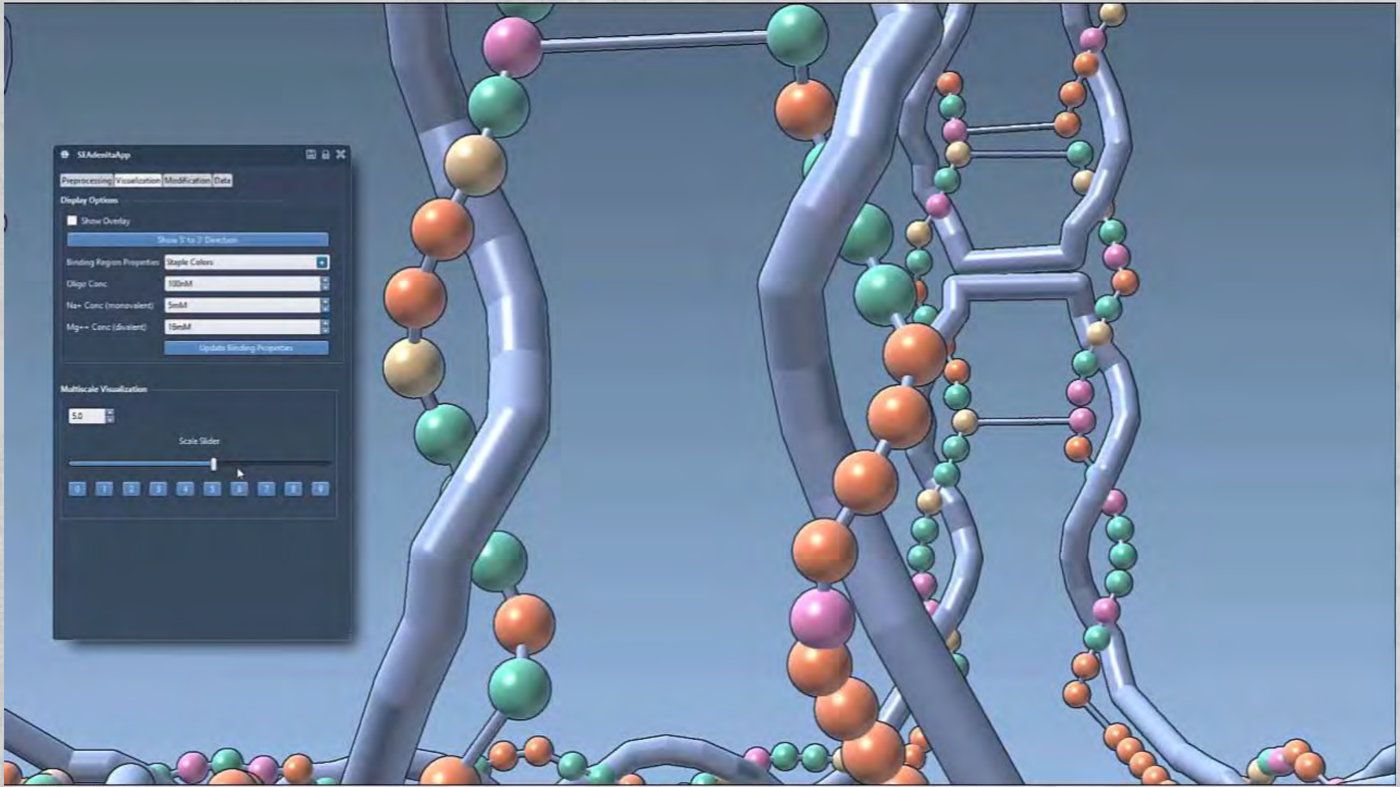
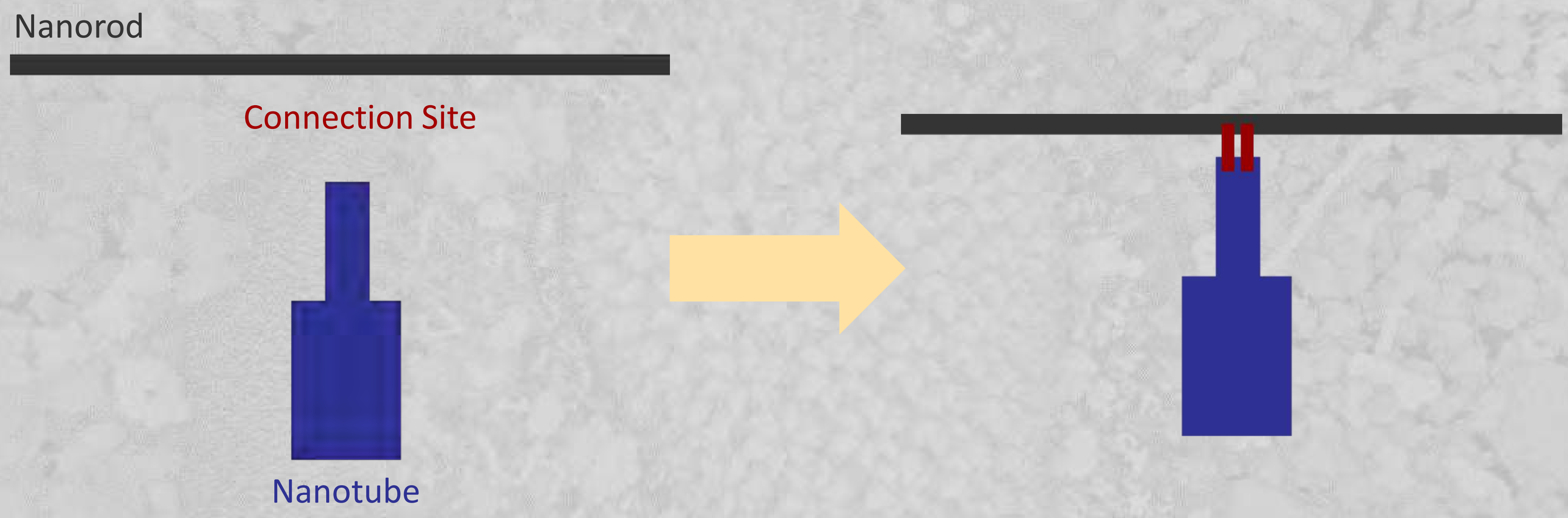
Task: Crossovers



Case Study | Connecting Nanotube with Nanorod



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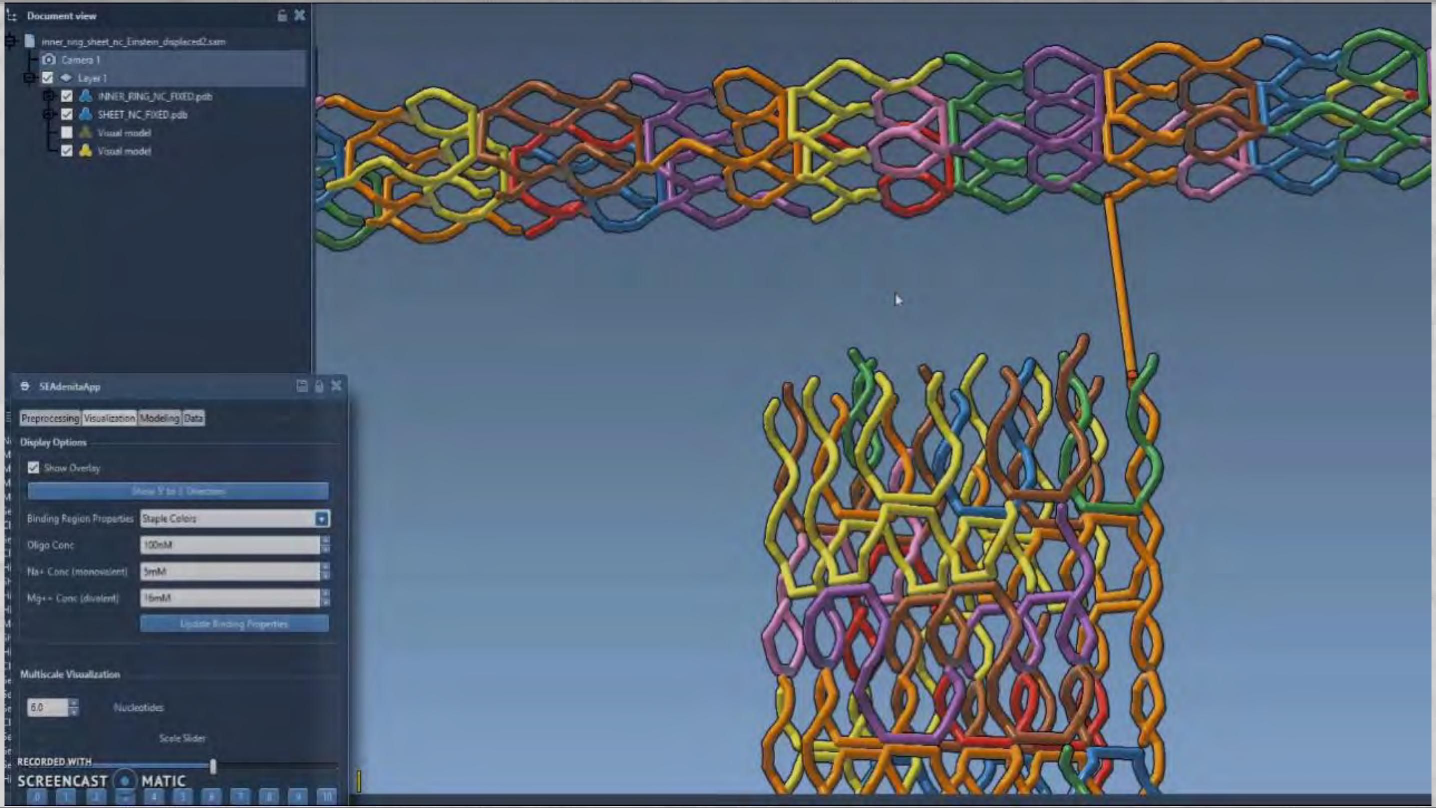
Case Study | Connecting Nanotube with Nanorod



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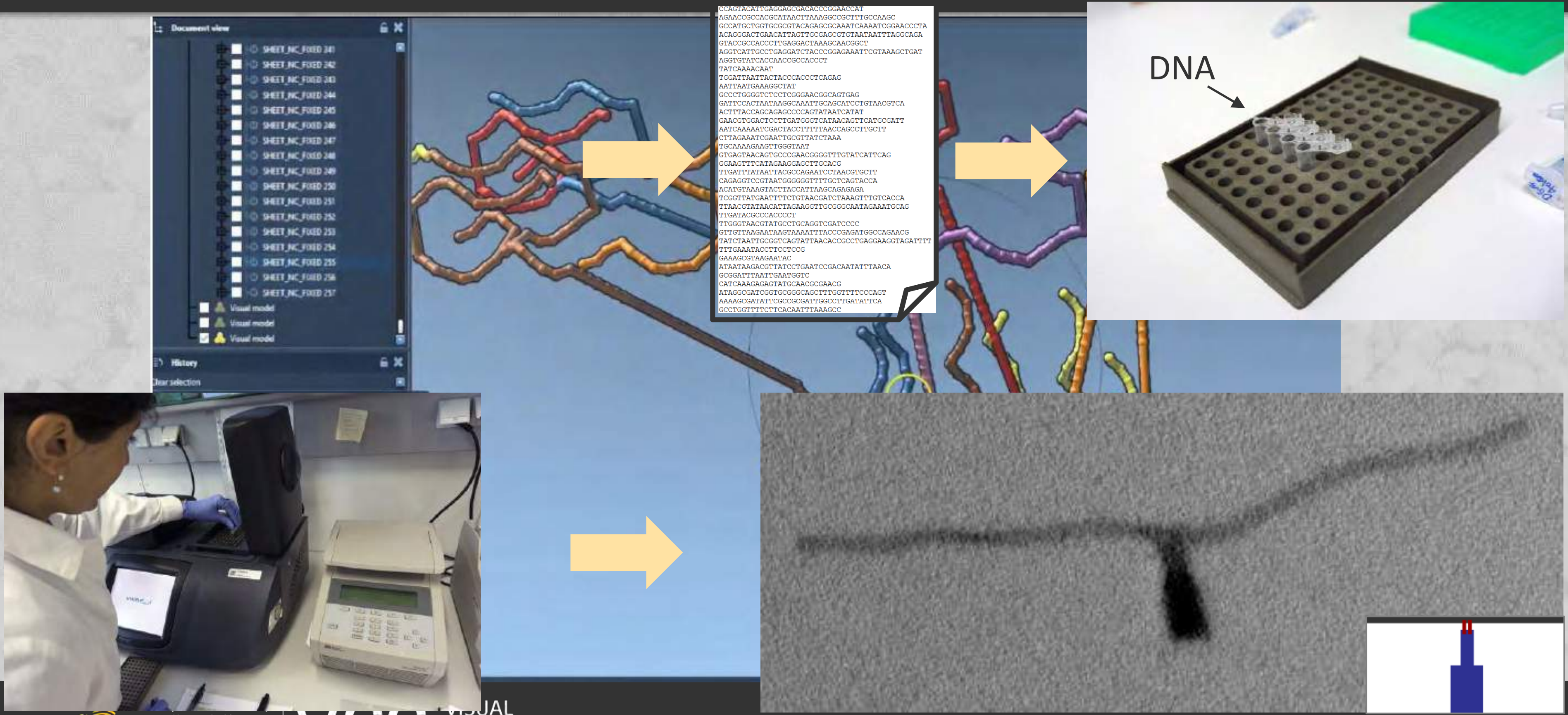
Case Study | In Vitro Experiment



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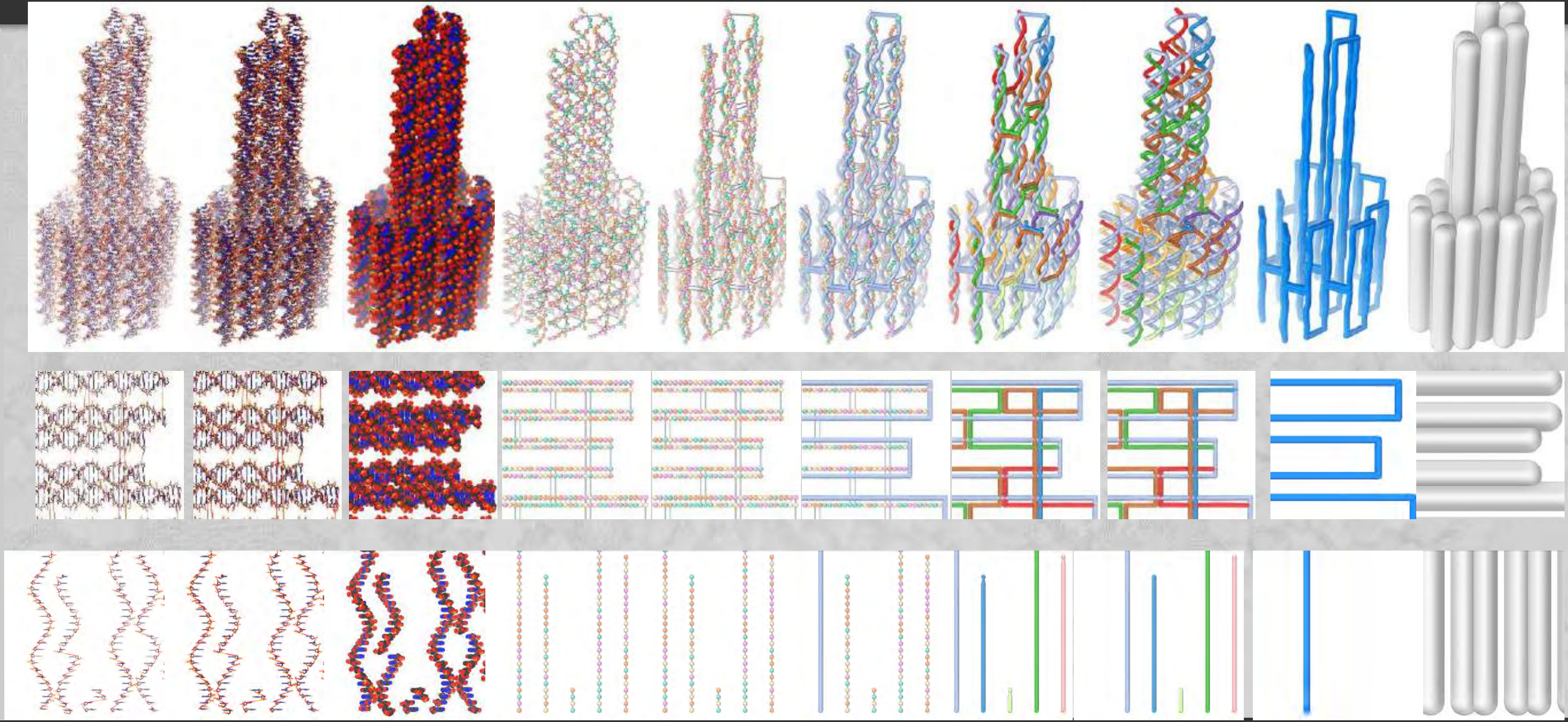
Dimension and Scale



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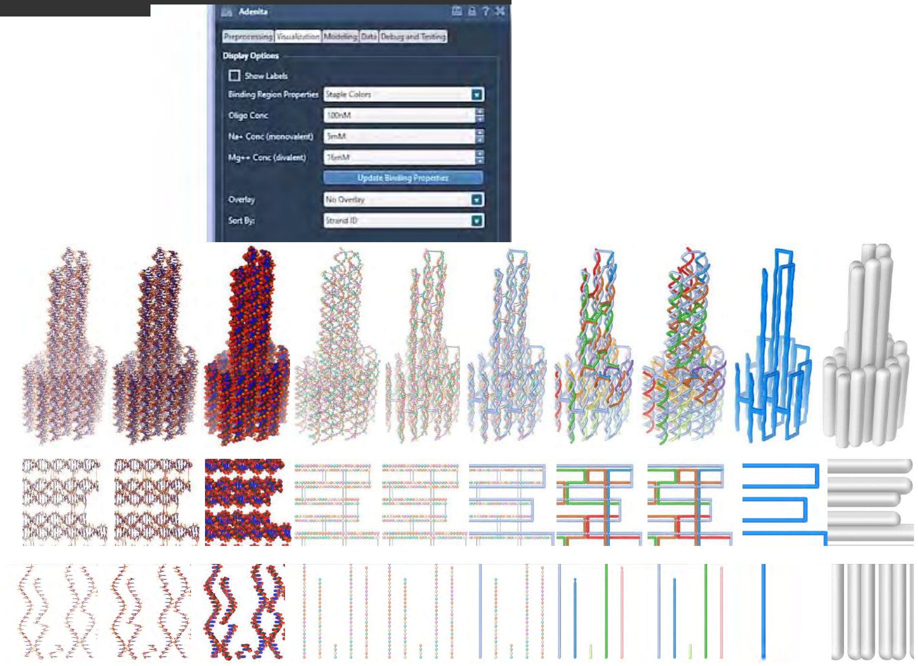
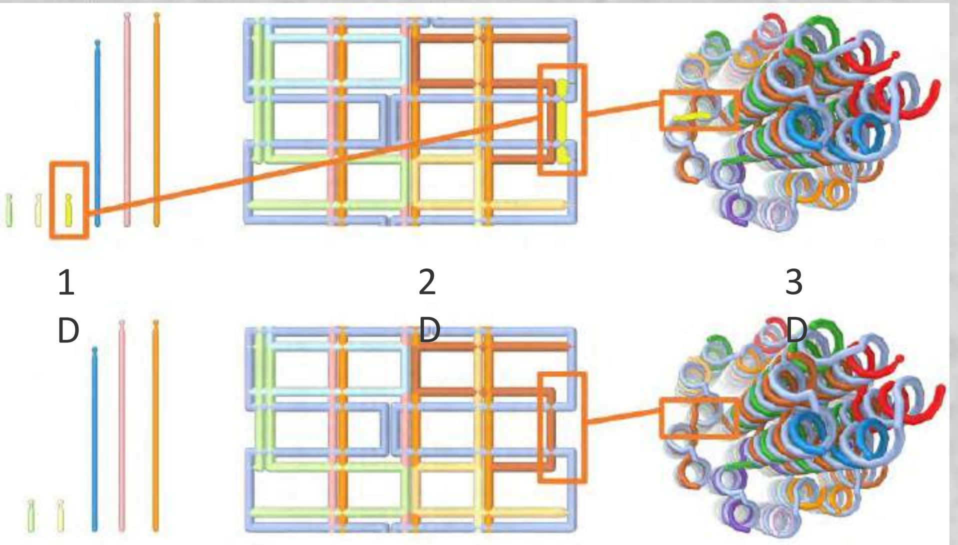
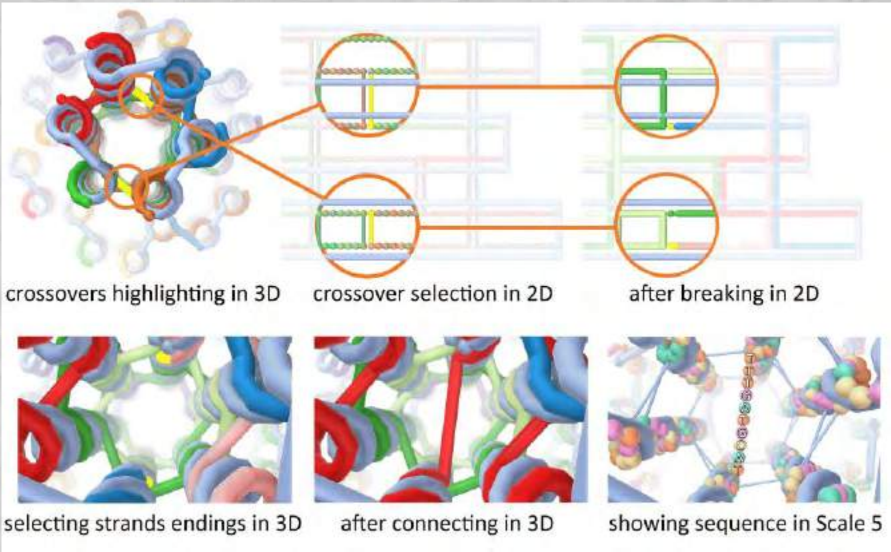
Dimension and Scale Unifying Map (DimSUM)



Abstraction-adaptive Modifications



Task 1: Removing Short Staple Strands



Task 2: Adding Bridging Strands

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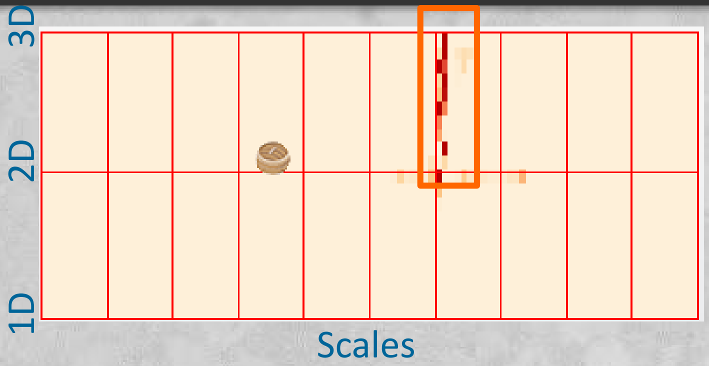
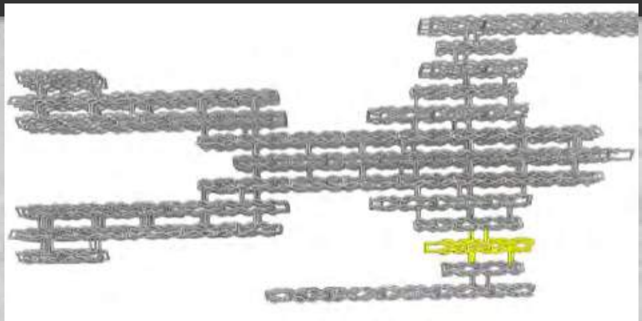
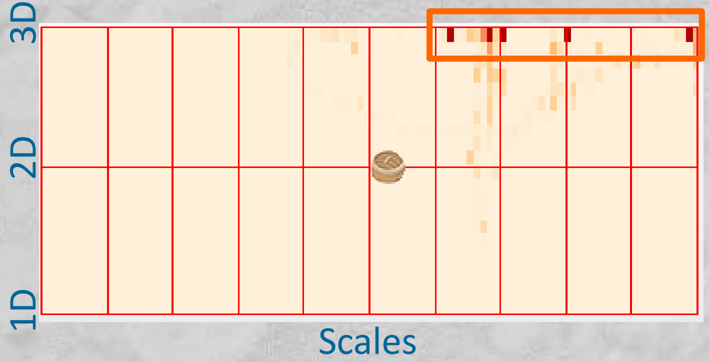
Case Studies



Case study 1

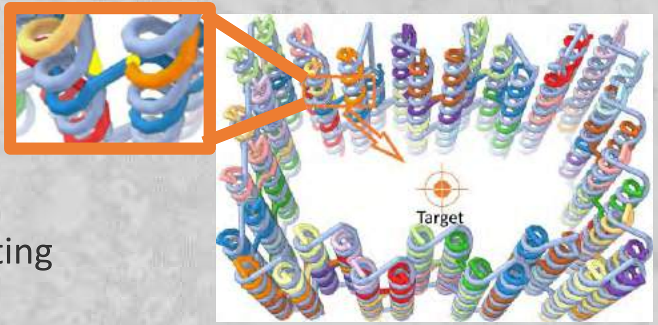
- Domain scientist 1
- Structural motif design
- Transition 3D to 2D





Case study 2

- Domain scientist 2
- Surface strand analysis
- 3D scales most interesting



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GUIDANCE

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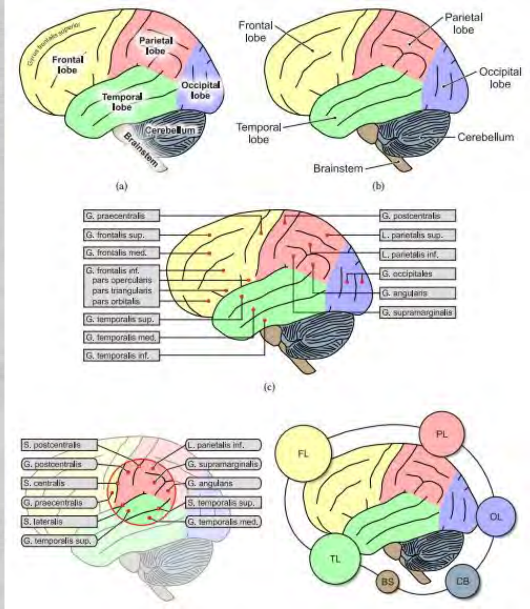
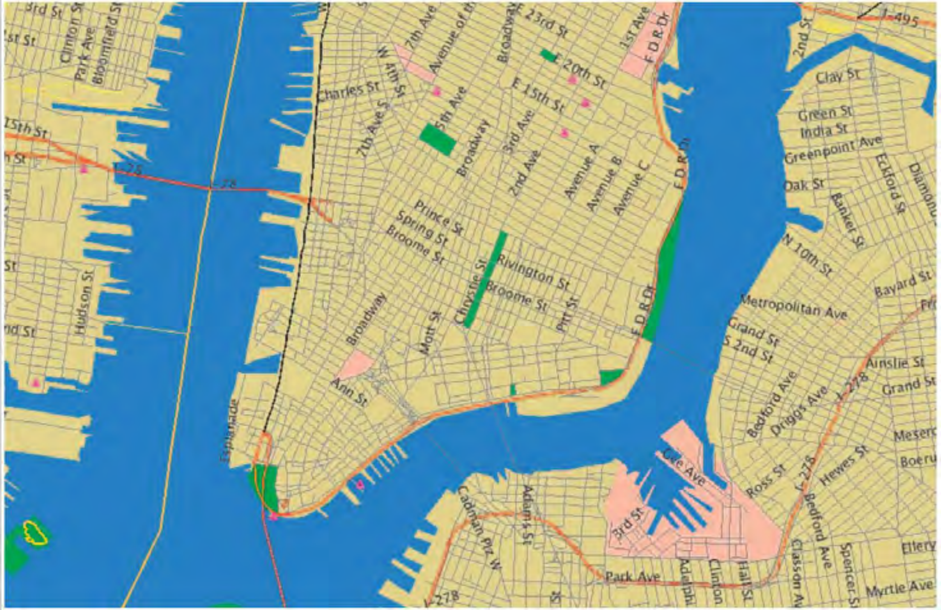
VCC VISUAL COMPUTING CENTER

Ivan Viola

Interactive Labeling

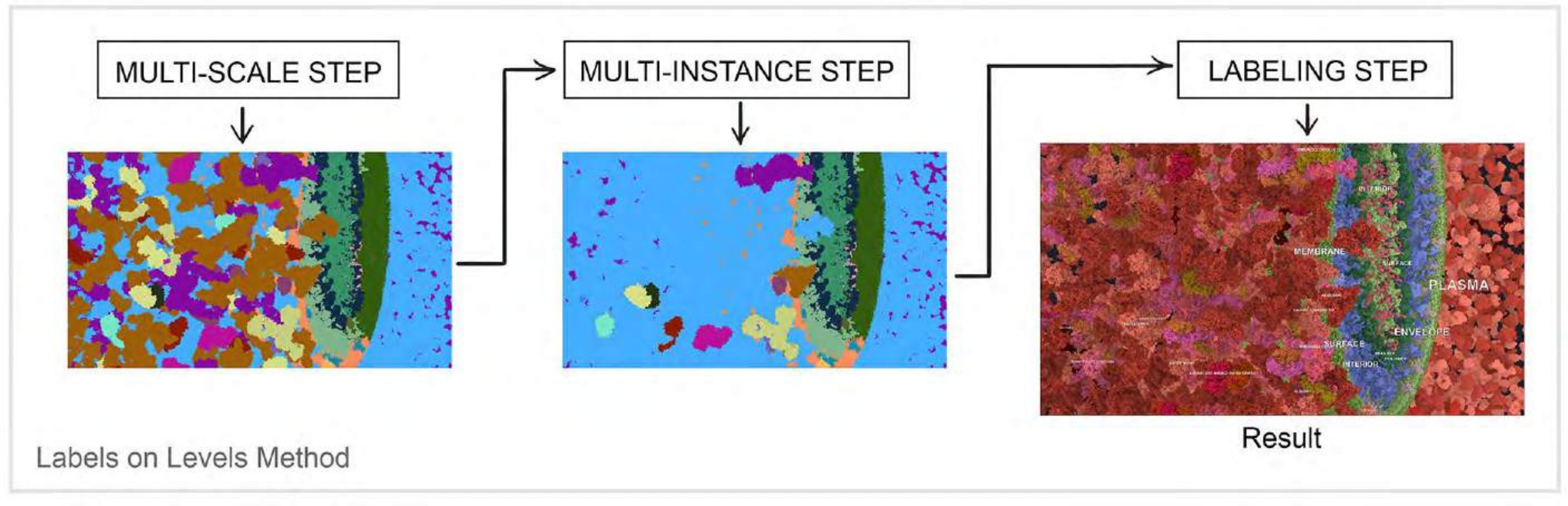


[Oeltze-Jafra and Preim 2014]



[Been et al. 2006]

Labels on Levels Algorithm

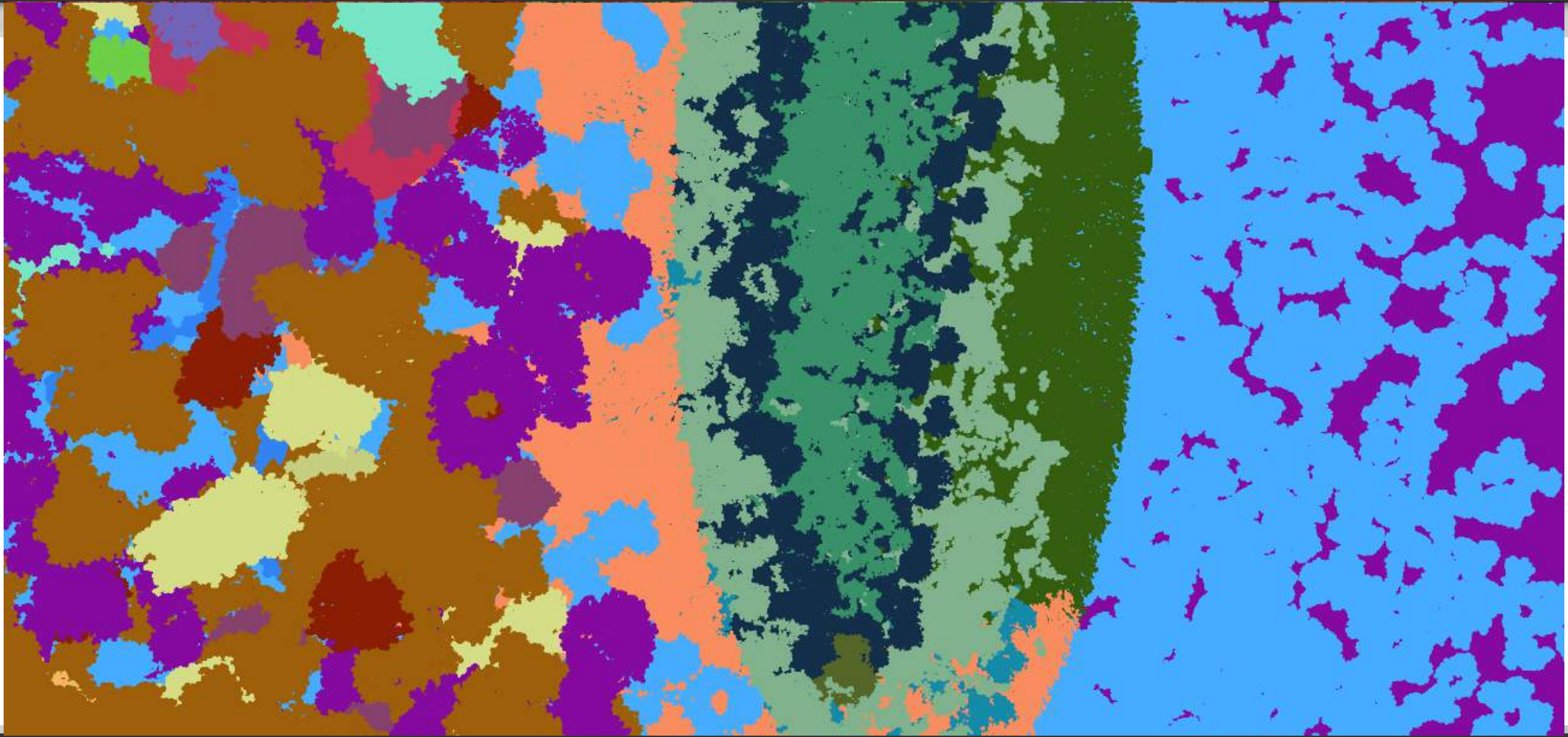


Multi-Scale Step

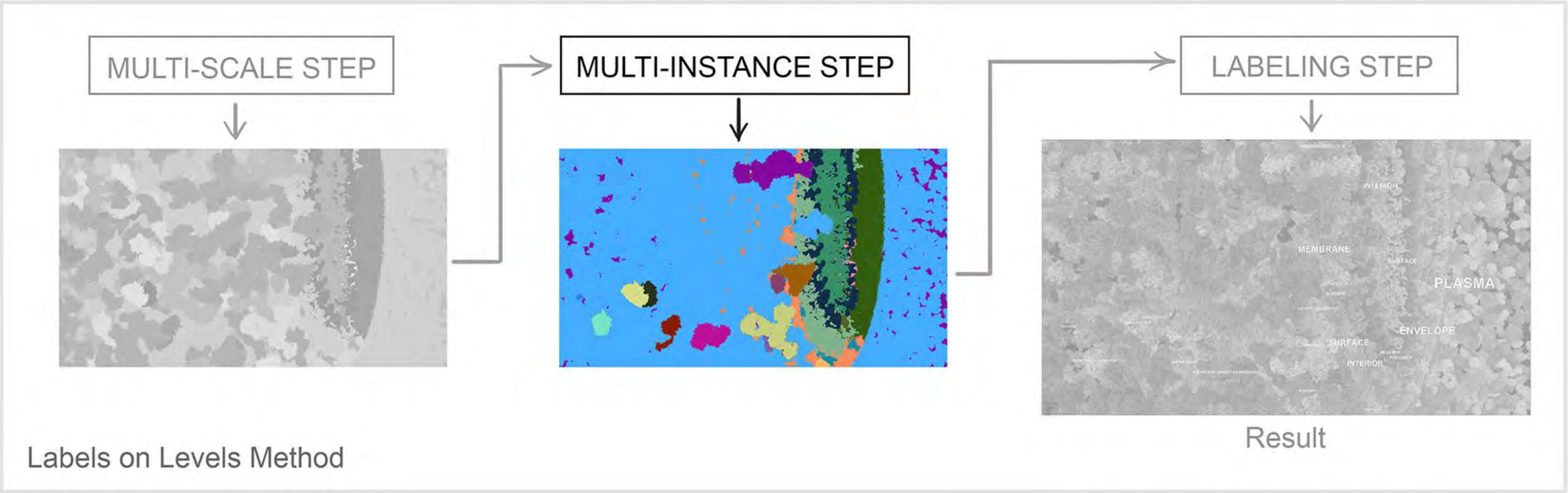
Multi-Scale Step

capsid protein → hexamer → capsid → HIV

Multi-Scale Step

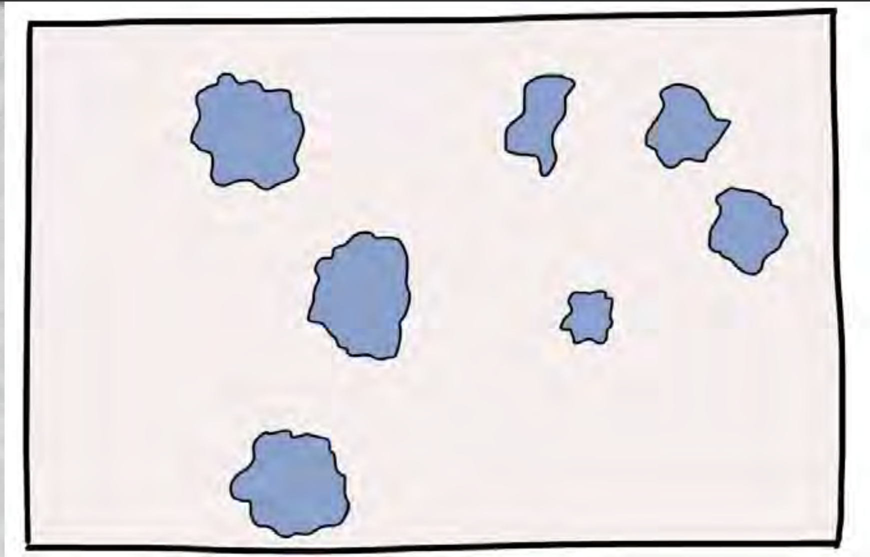


Multi-Instance Step



Multi-Instance Step

- Choose a representative
- Evaluate 4 criteria
  - Prominence criterion
  - Distance criterion
  - Border criterion
  - Temporal coherence criterion
- Output: 2D positions of label anchors



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Multi-Instance Step

- Choose a representative
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  - Prominence criterion
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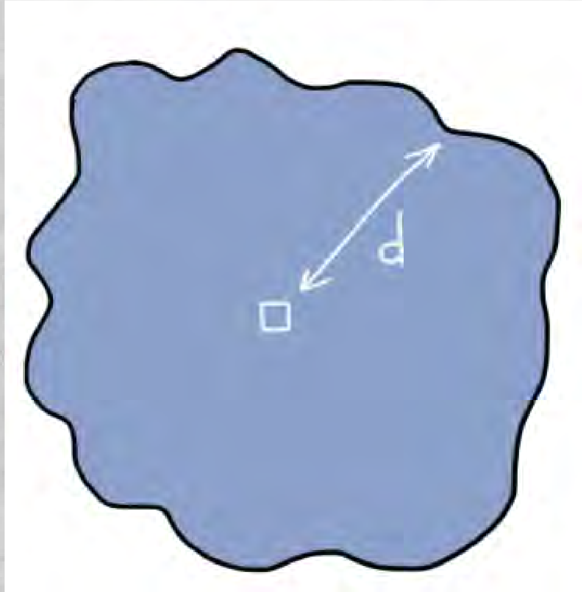

Multi-Instance Step

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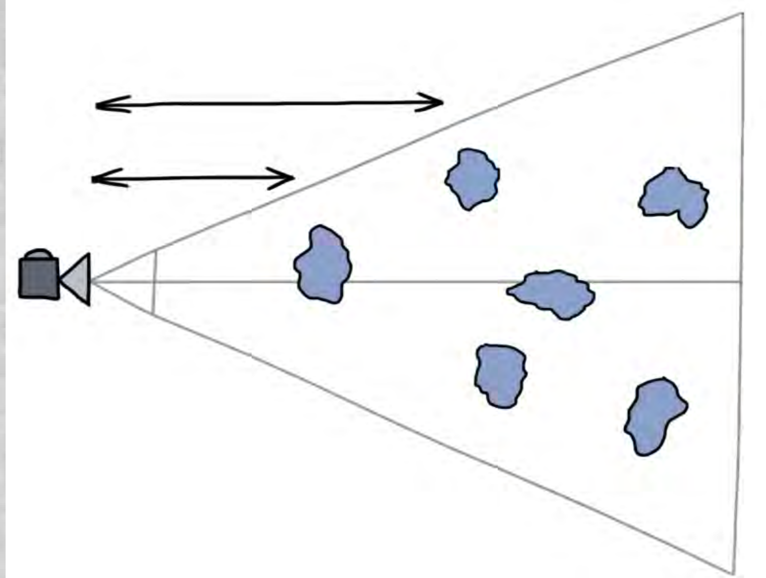

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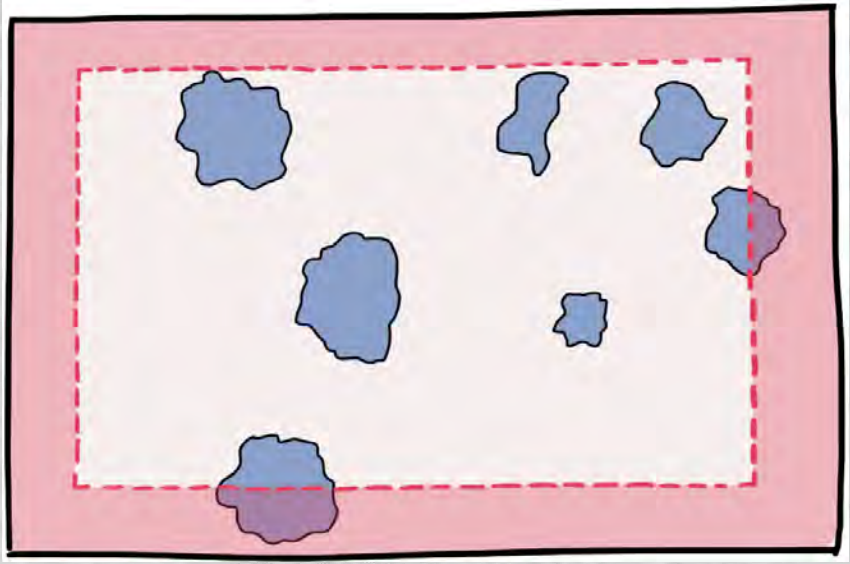

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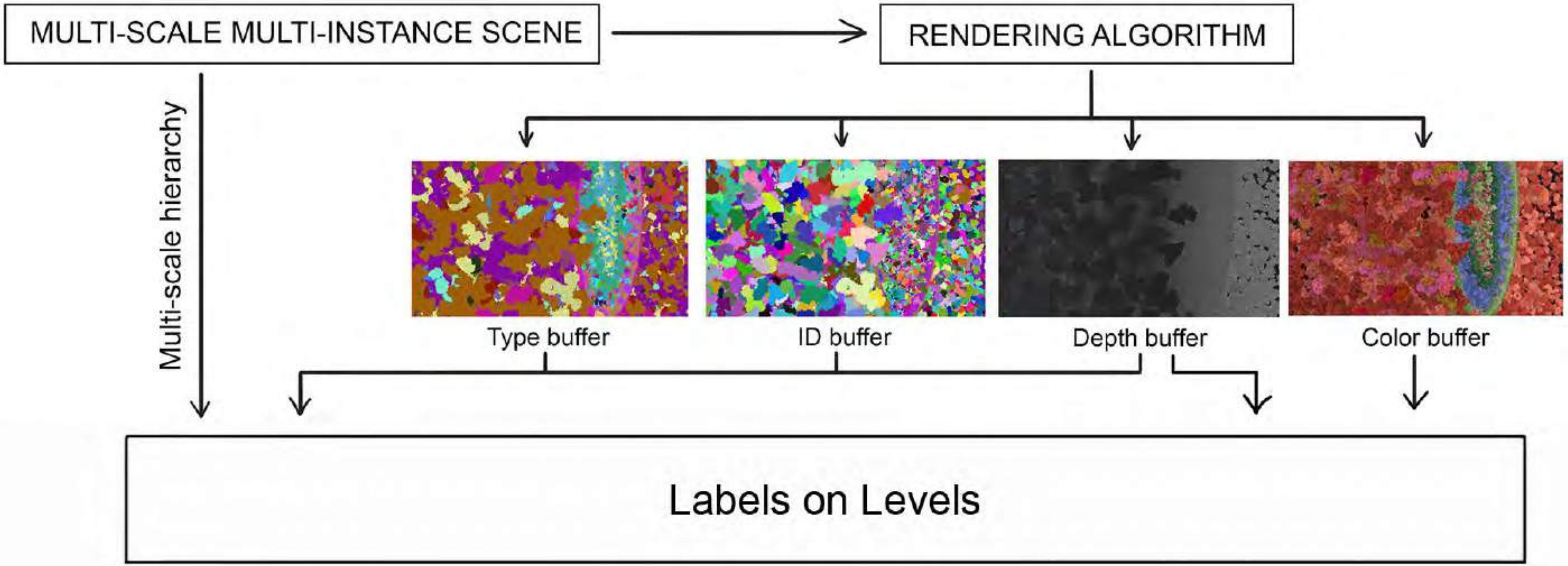
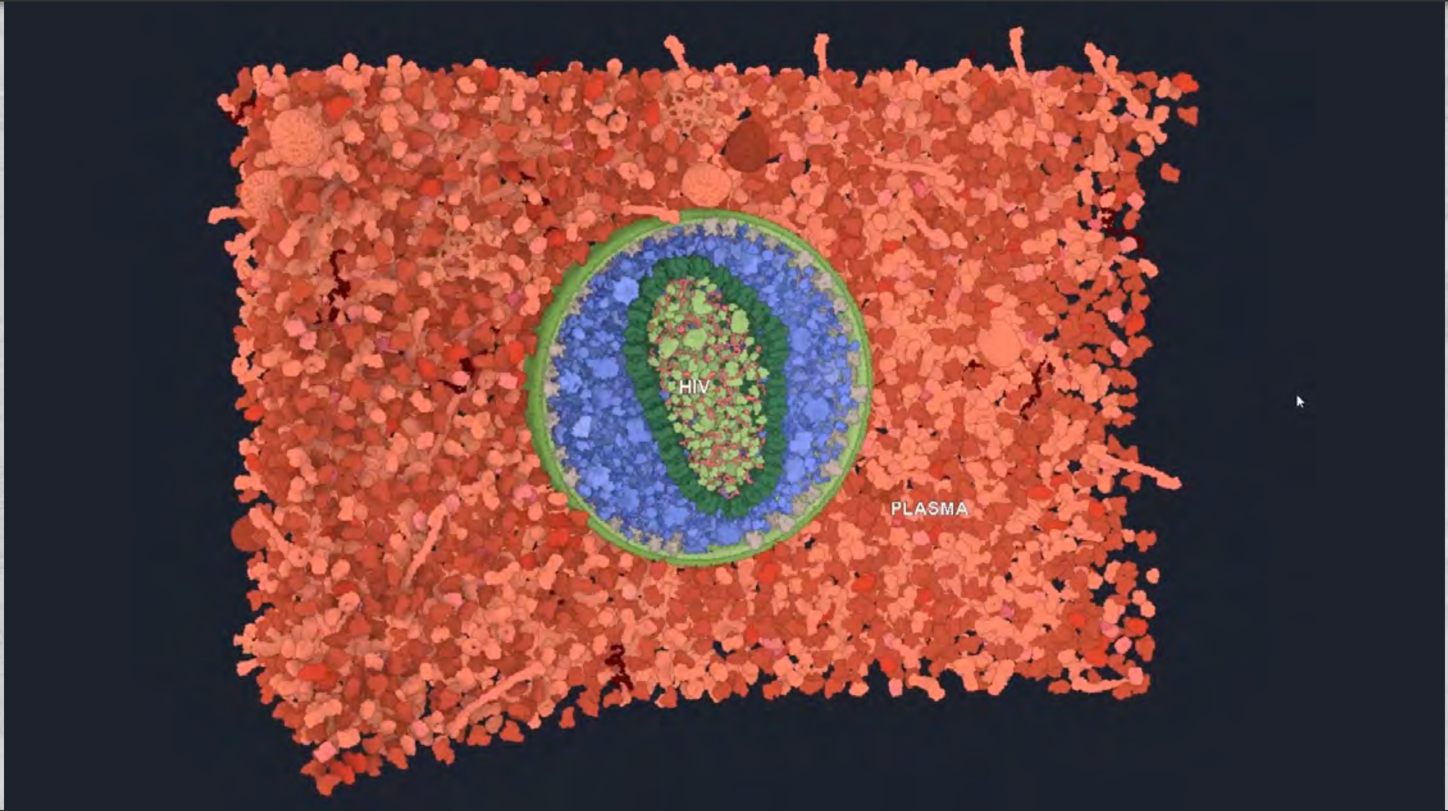
Multi-Instance Step

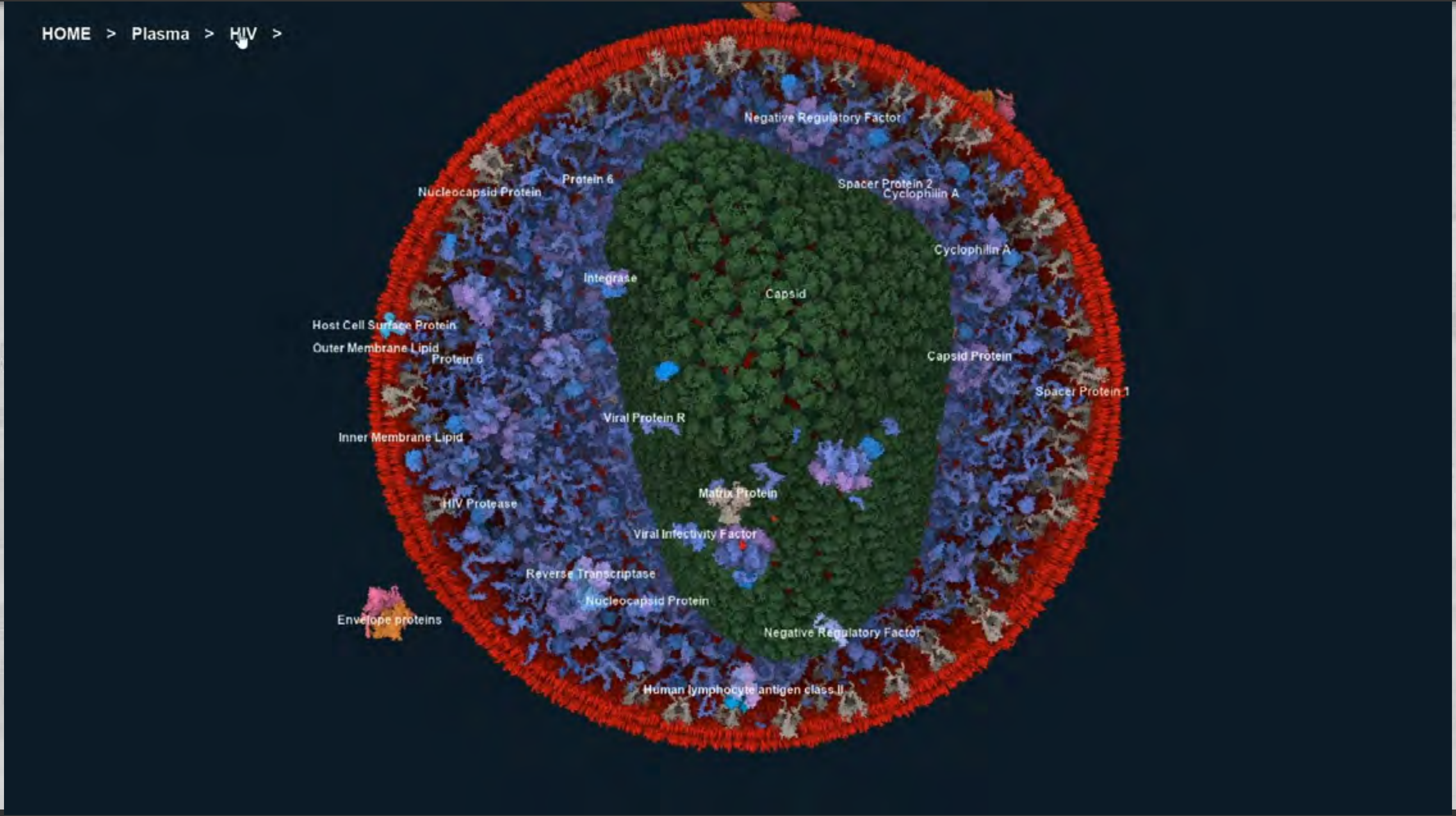
Image-Space Technique



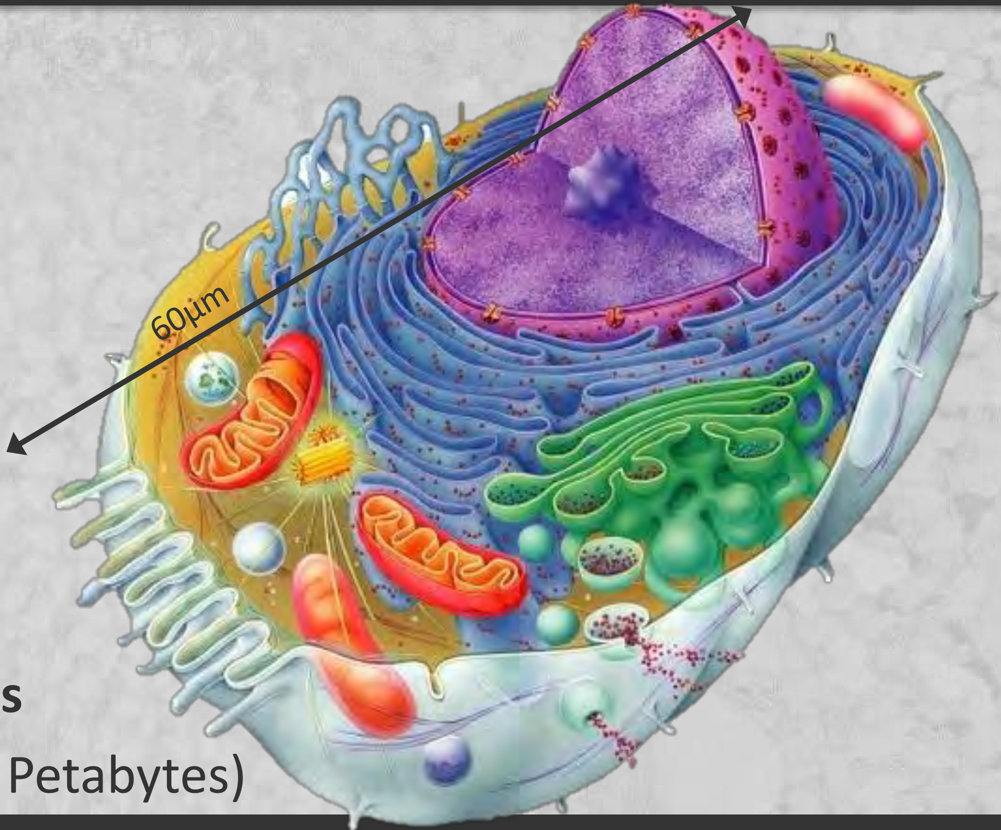
Multi-Scale and Multi-Instance Labeling



Multi-Scale Navigation through Labeling



Integrating Mesoscale and Cellscale



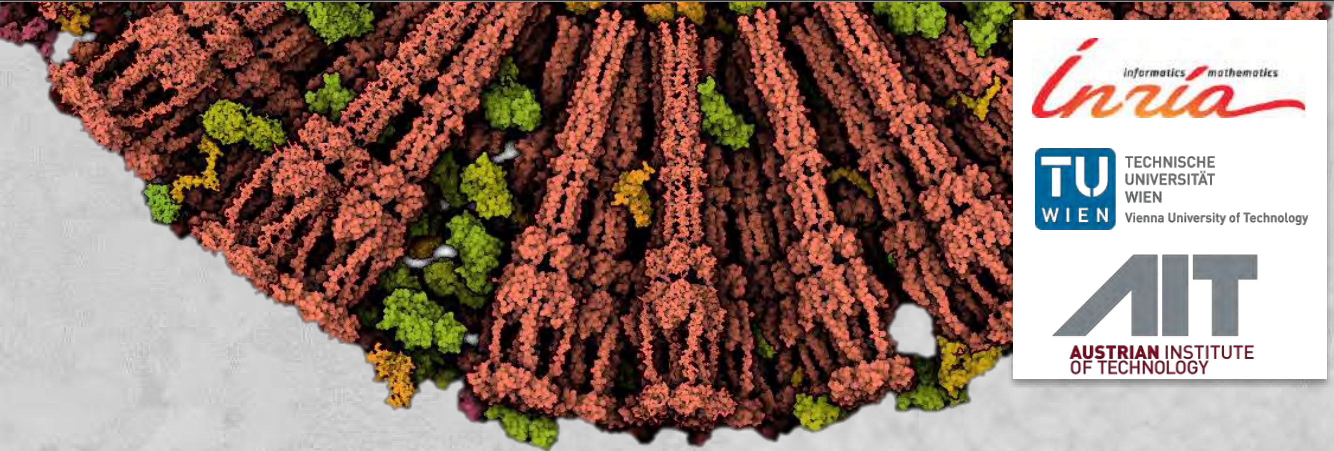
100,000,000,000,000 atoms

(1,600,000,000,000,000 bytes = 1.6 Petabytes)

Research Focus: Interactive Visual Cell

KAUST

Thank you for your attention!



Inria informatics mathematics

TU WIEN TECHNISCHE UNIVERSITÄT WIEN Vienna University of Technology

AIT AUSTRIAN INSTITUTE OF TECHNOLOGY

THE SCRIPPS RESEARCH INSTITUTE

ALLEN INSTITUTE for CELL SCIENCE

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