

Kolloquium

Visualization of molecule surface dynamics

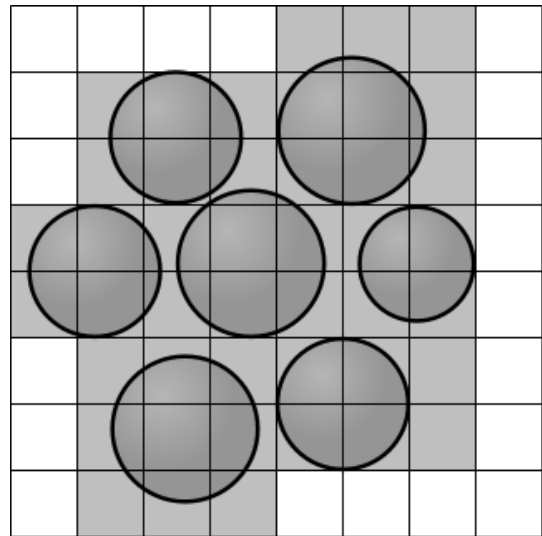
Contents

- Motivation
- Surface Extraction
- Ascension
- Layers
- Residue Surface-Proximity
- Evaluation
- Conclusion

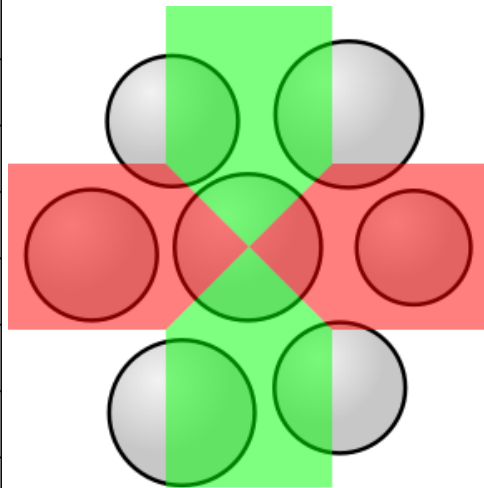
Motivation

- Surface of molecules defines binding behavior
- Folding simulation data hard to interpret
- Available software does not support scientists in **surface dynamics visualization and analysis**

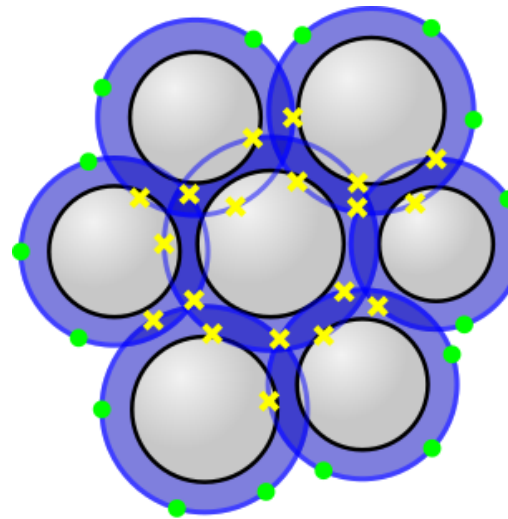
Surface Extraction Methods



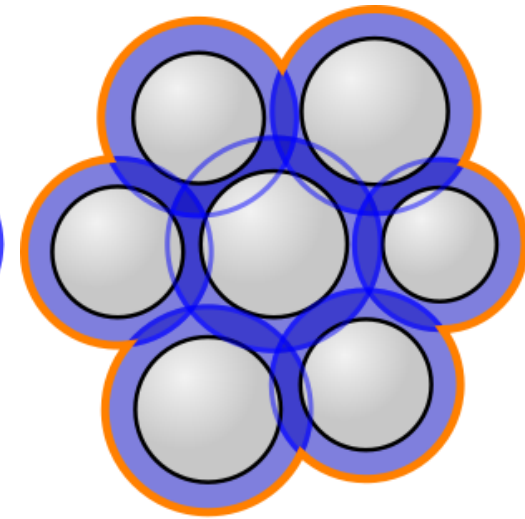
voxel-based



cylinder-based

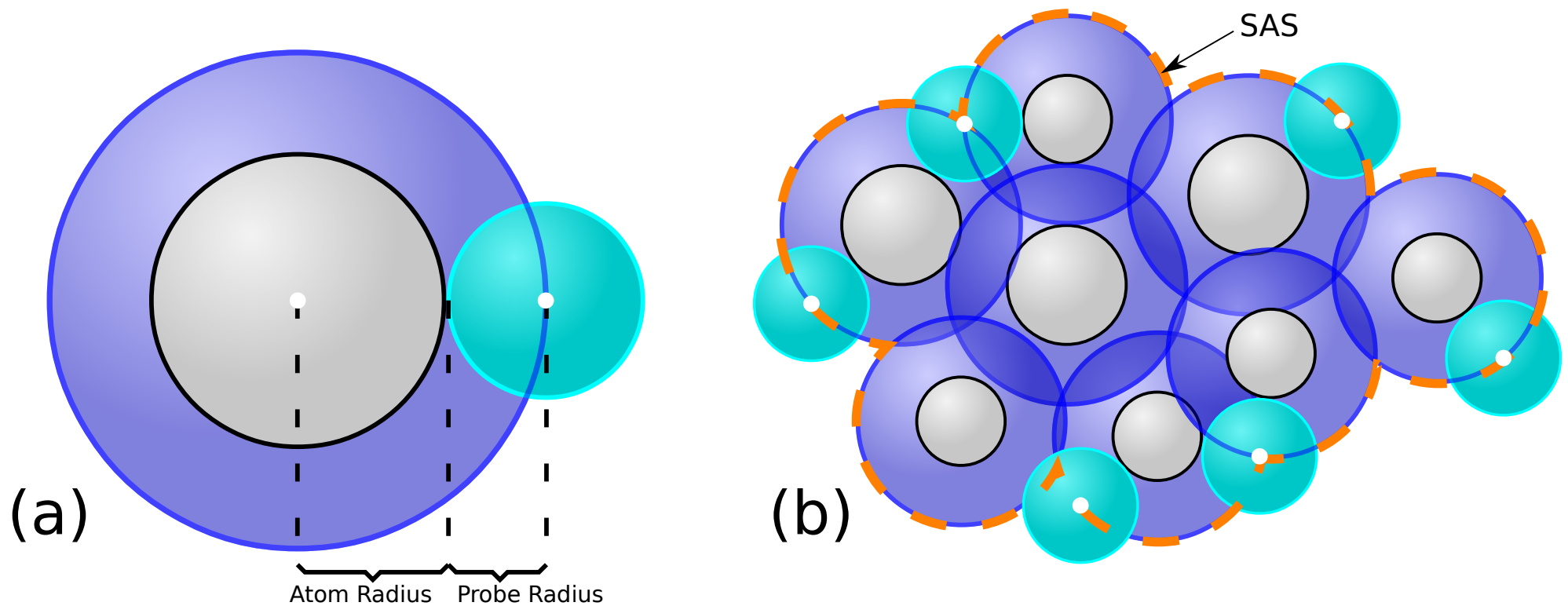


sample-based

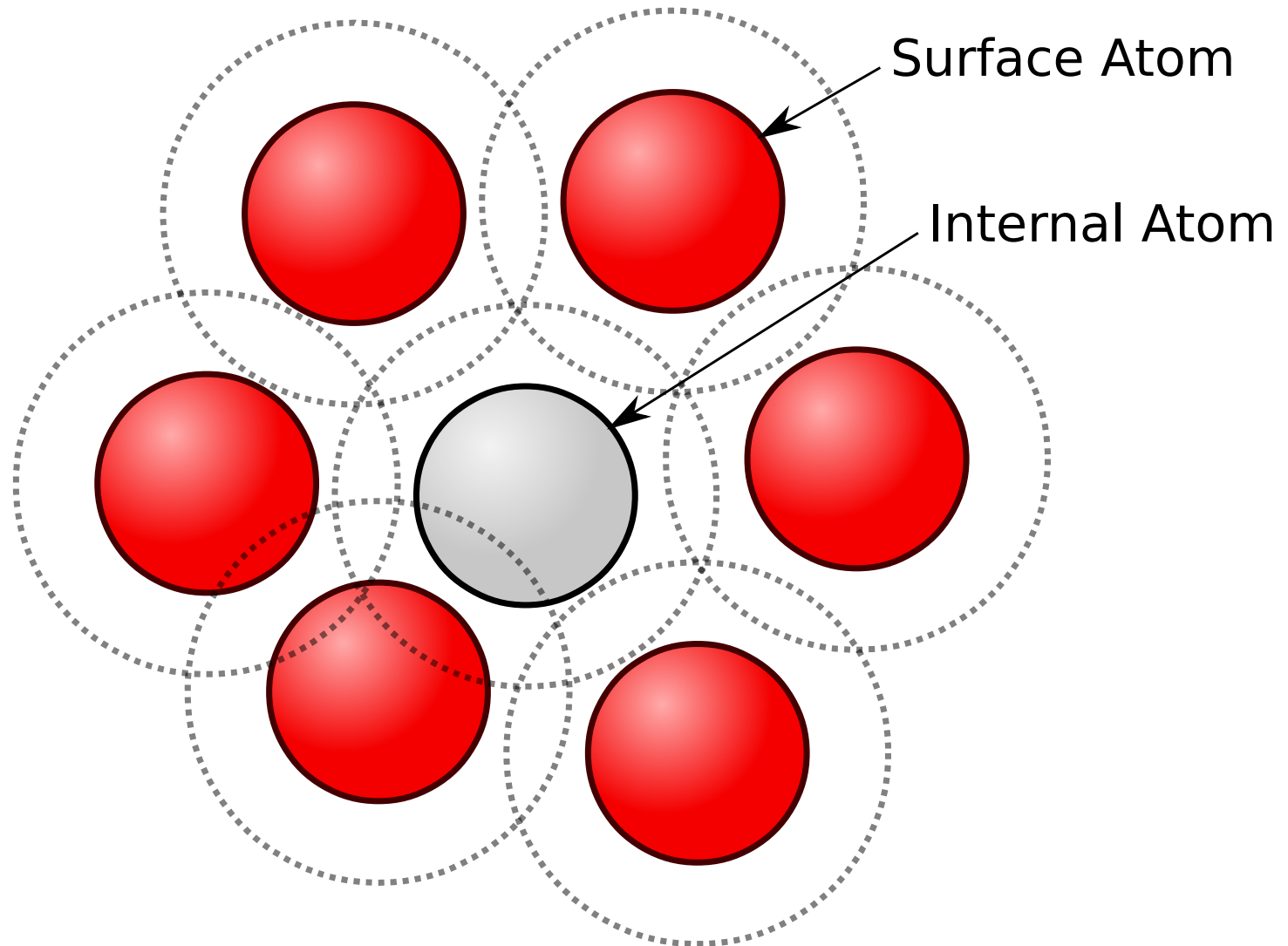


geometric-based

Solvent Accessible Surface

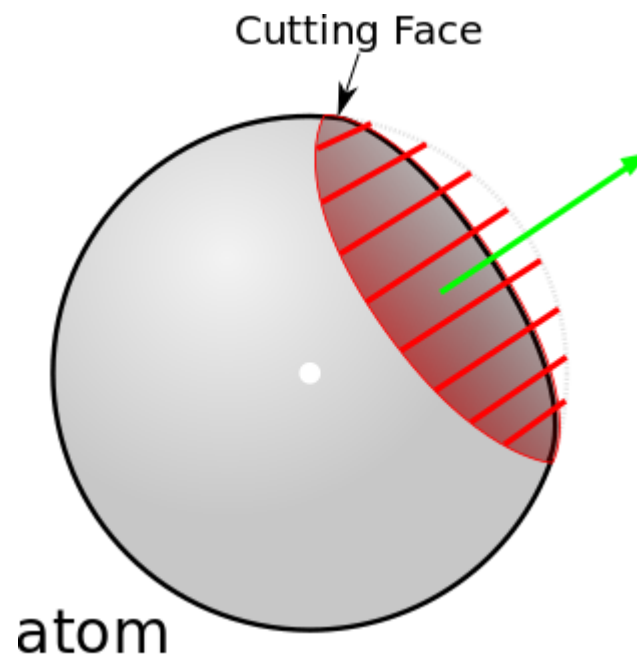
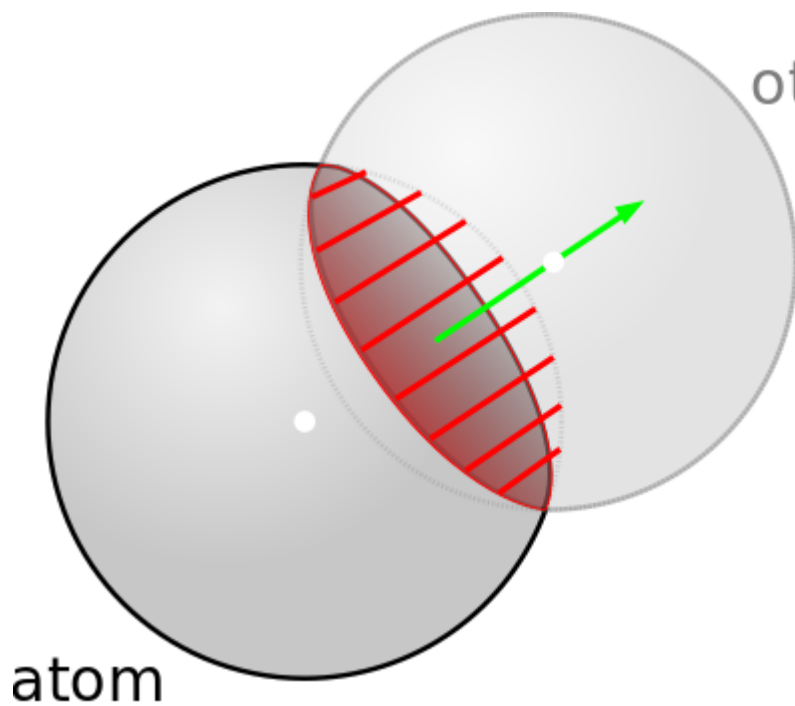
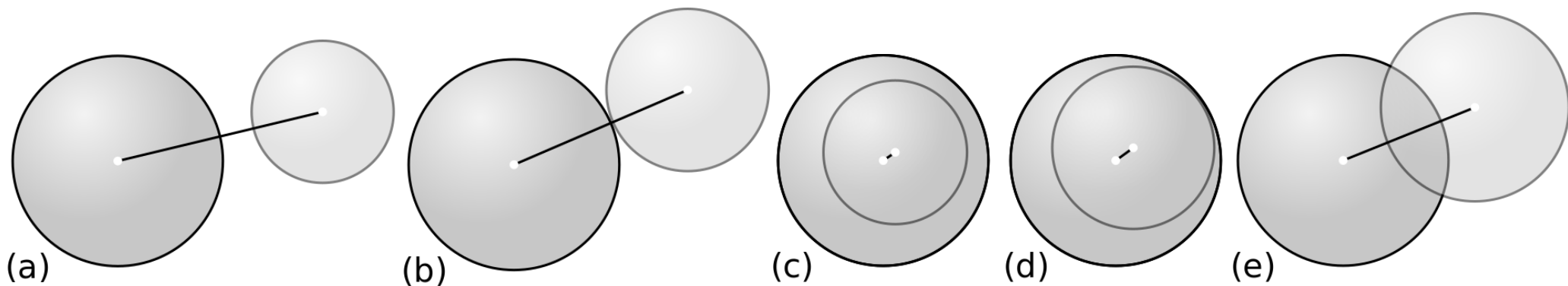


Surface Atom Extraction based on Extended Spheres



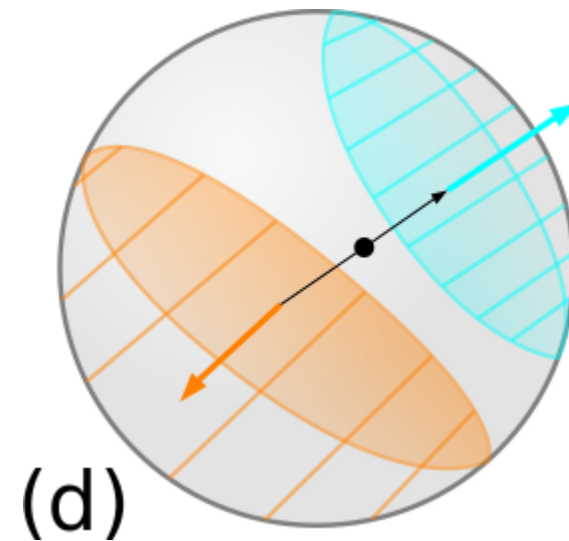
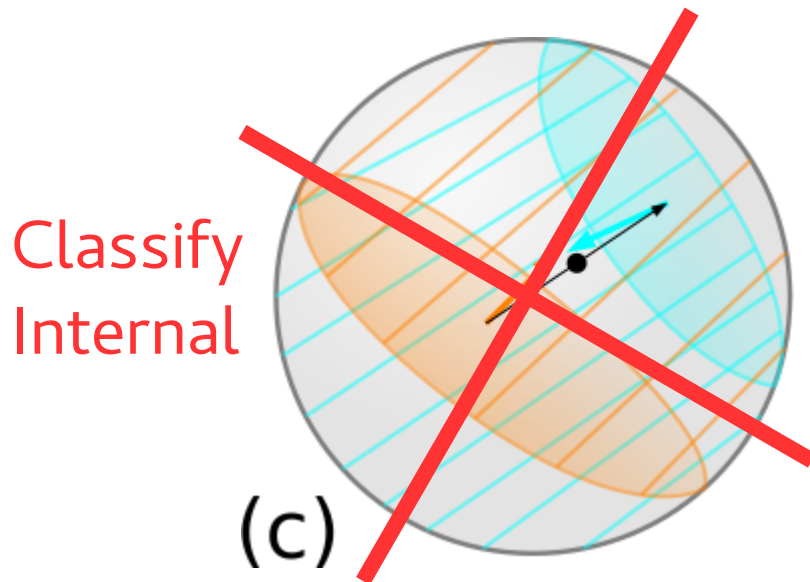
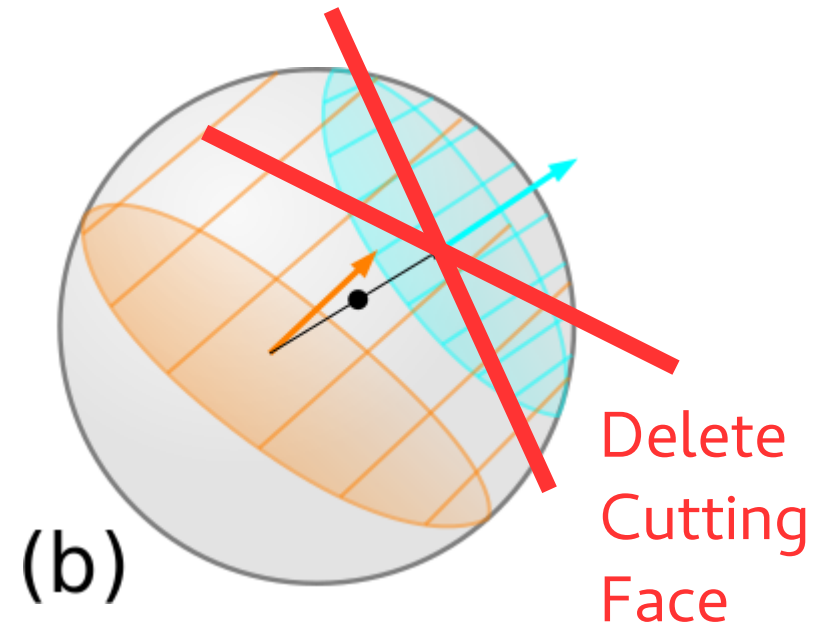
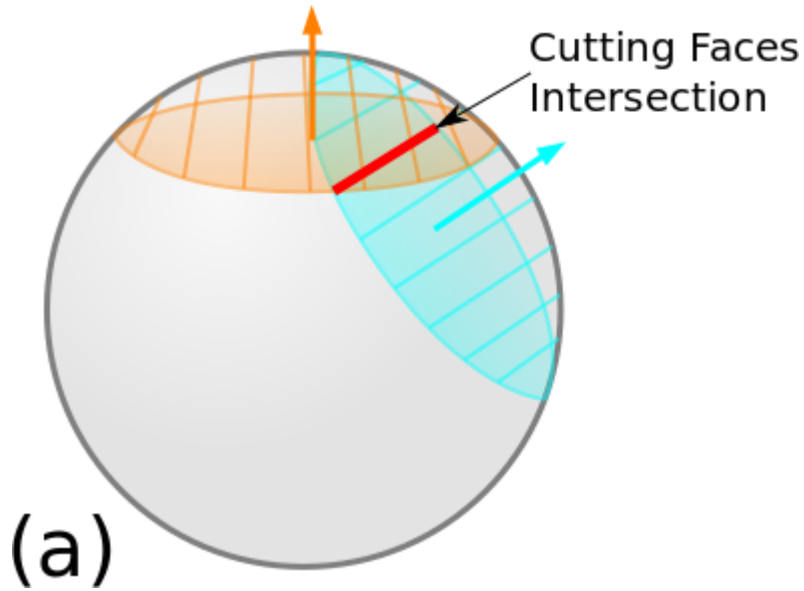
SAEES

Buildup of Cutting Face List



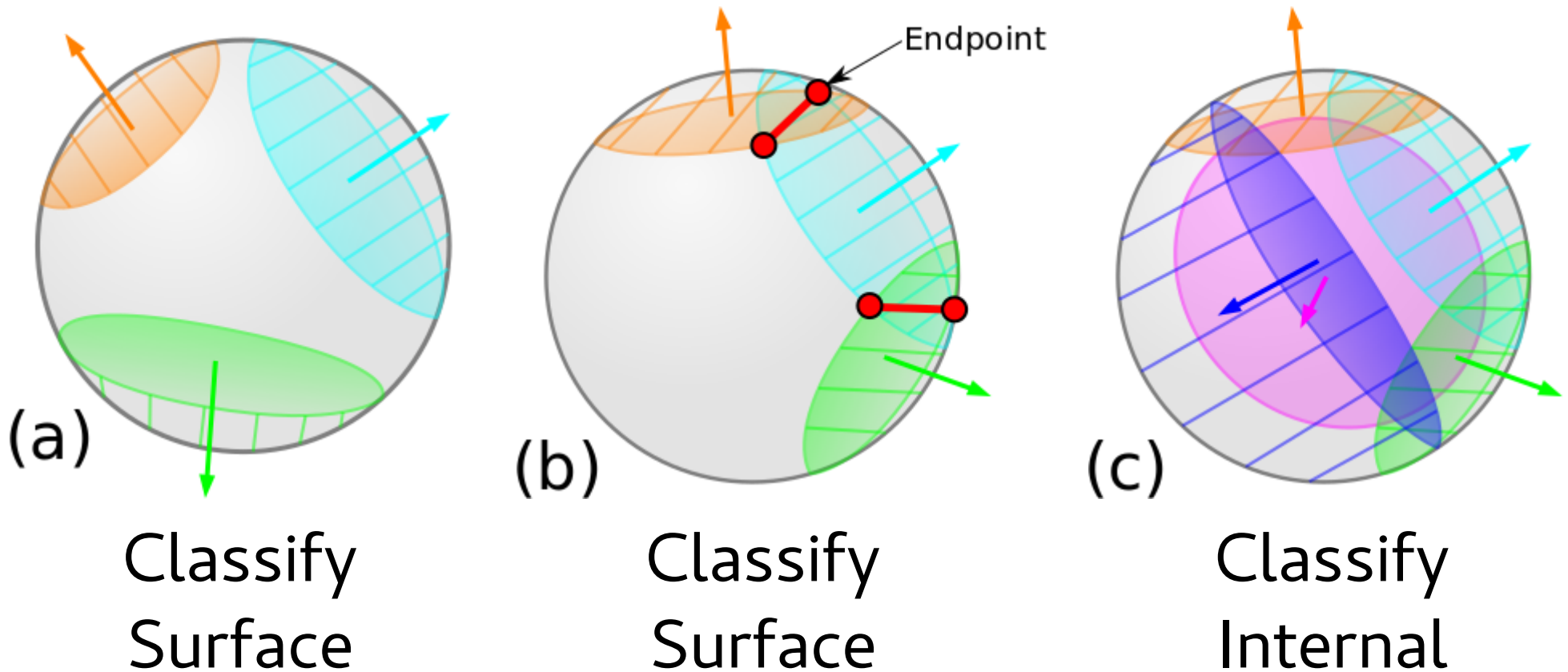
SAEES

Optimization of Cutting Face List



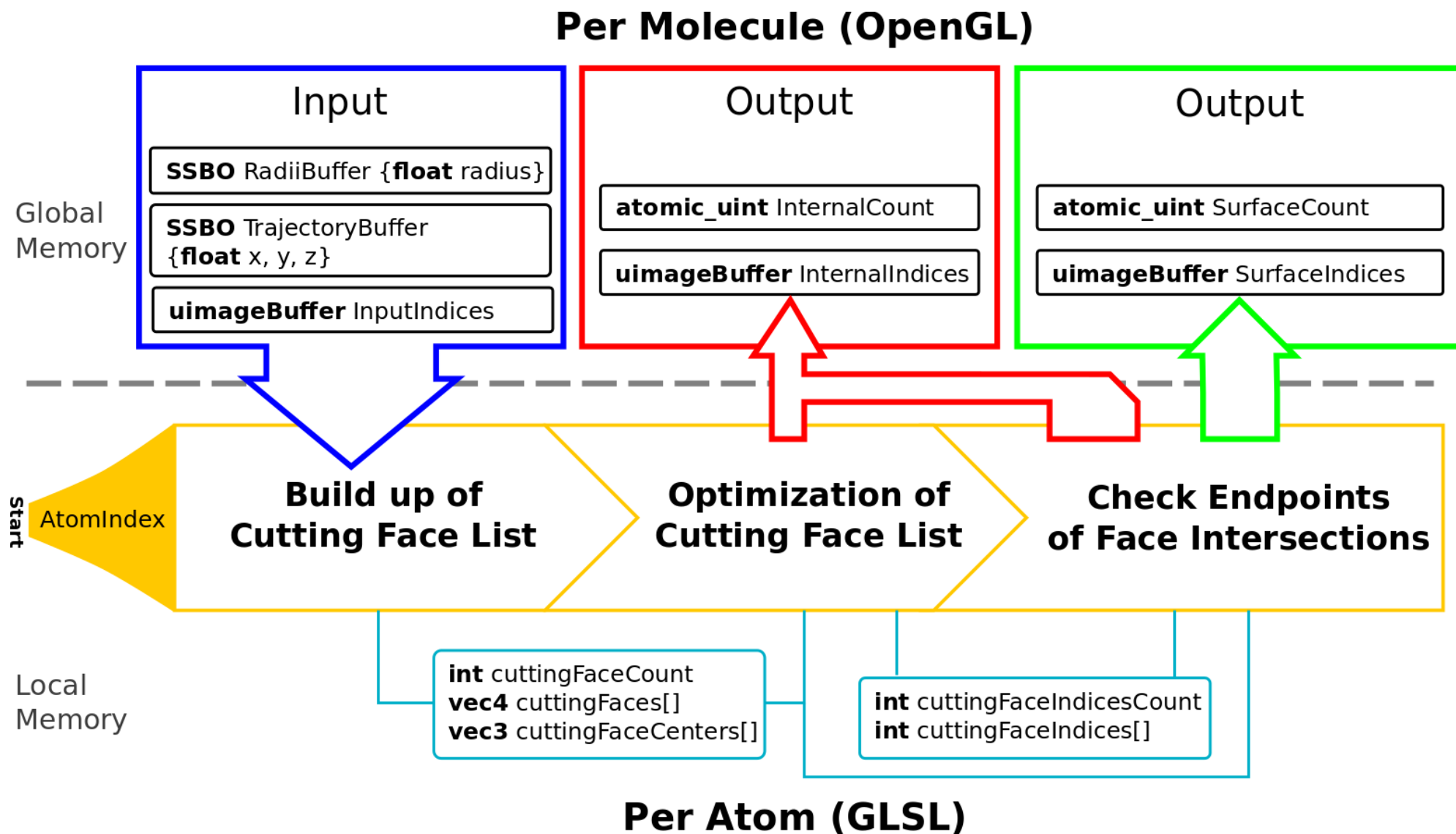
SAEES

Check Endpoint of Faces Intersections

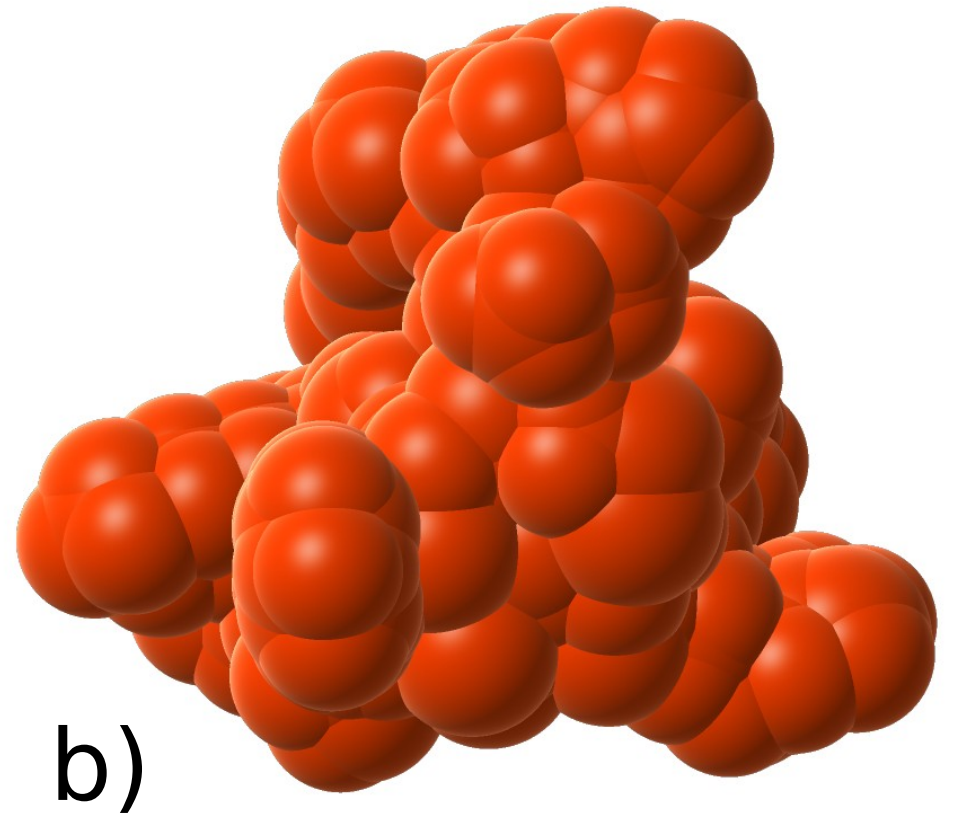
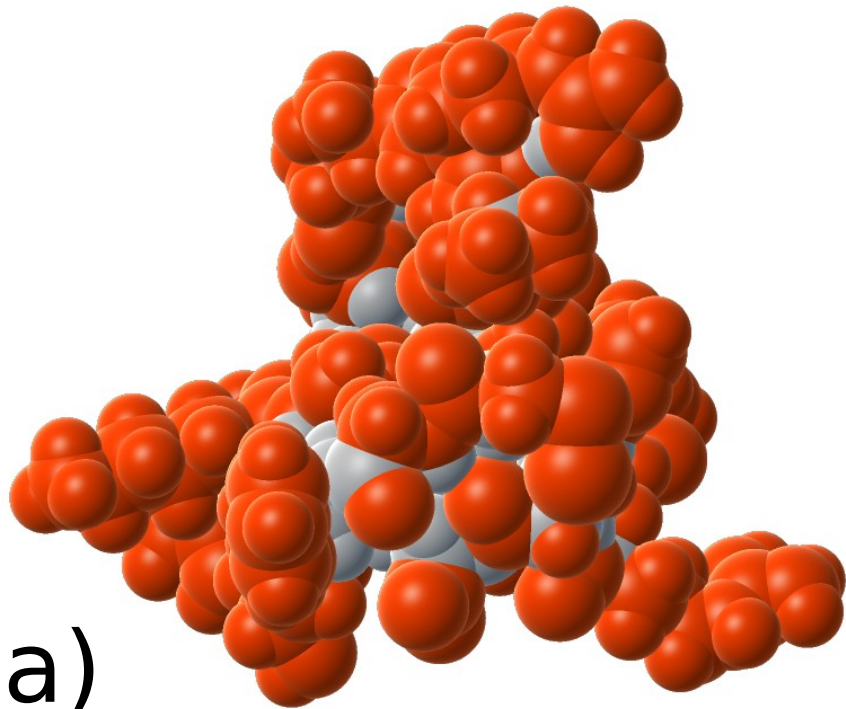


SAEES

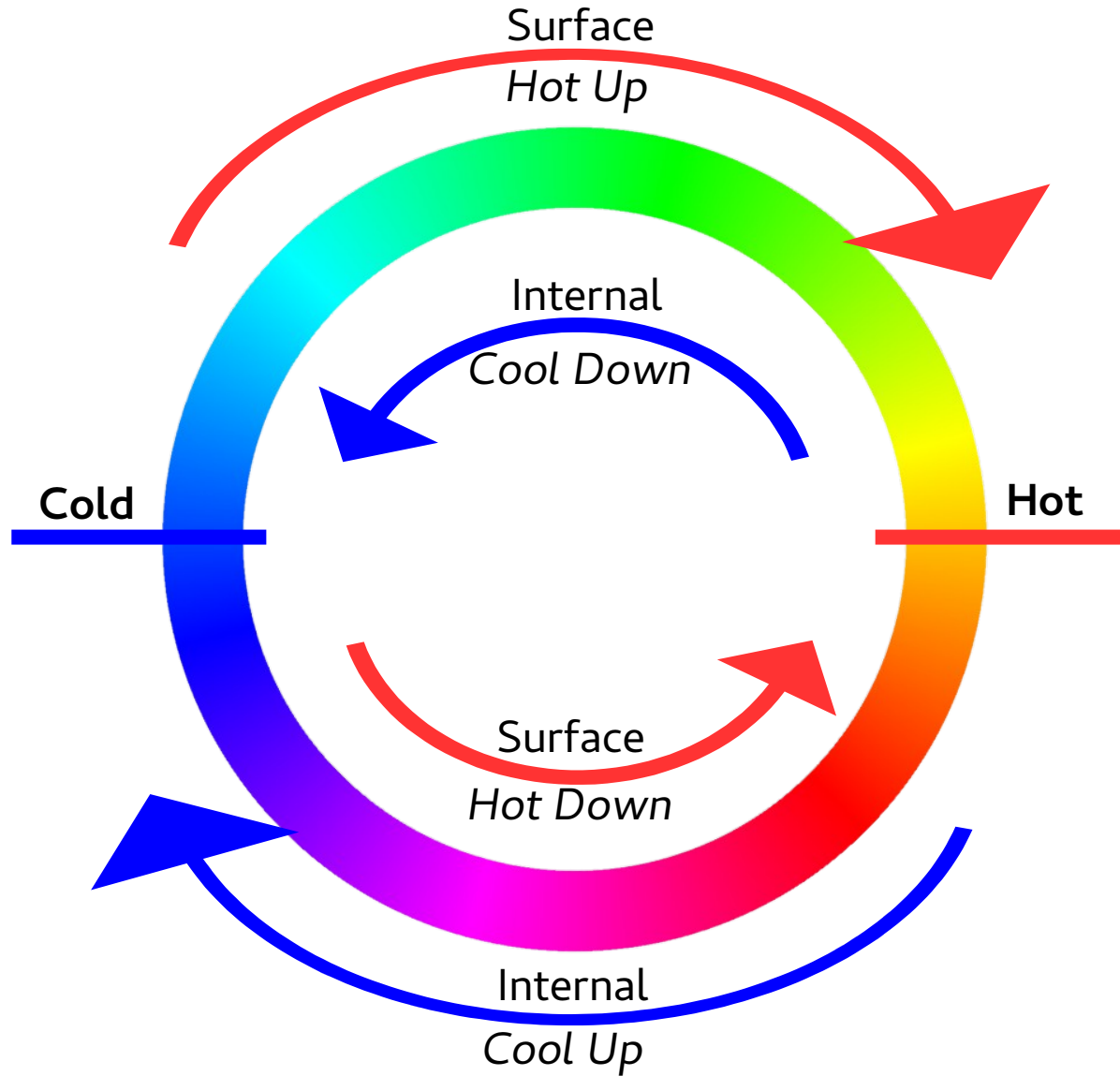
Compute Shader Program



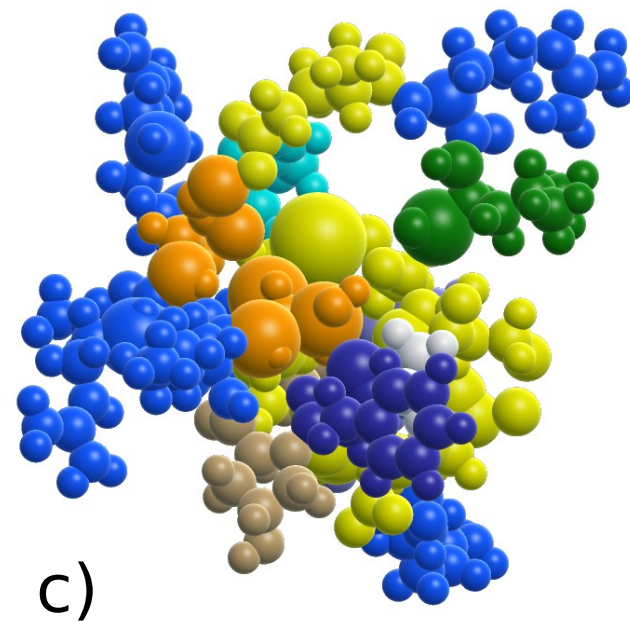
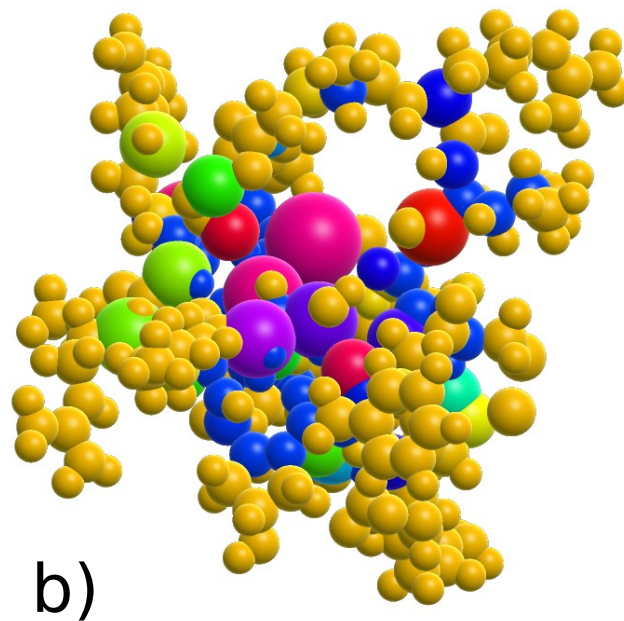
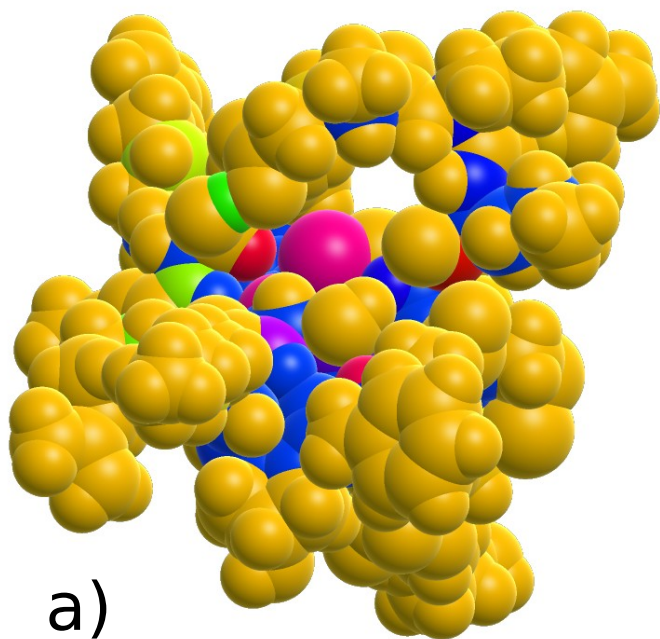
SAEES Results



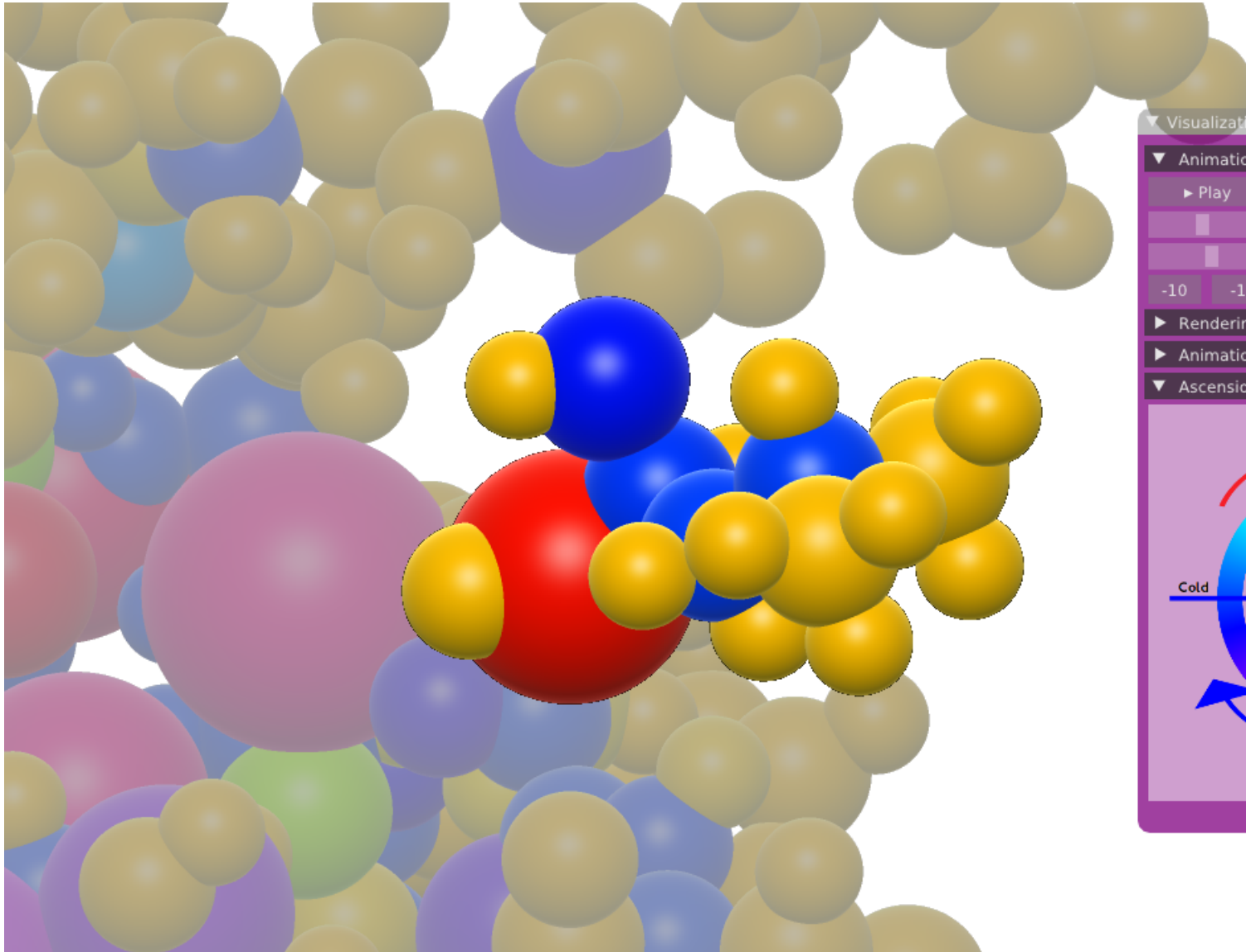
Ascension



Ascension Results



Ascension Results



Visualization

Animation

▶ Play Repeat

Rate

Frame

-10 -1 +1 +10

▶ Rendering

▶ Animation Smoothing

Ascension Helper

Surface Hot Up

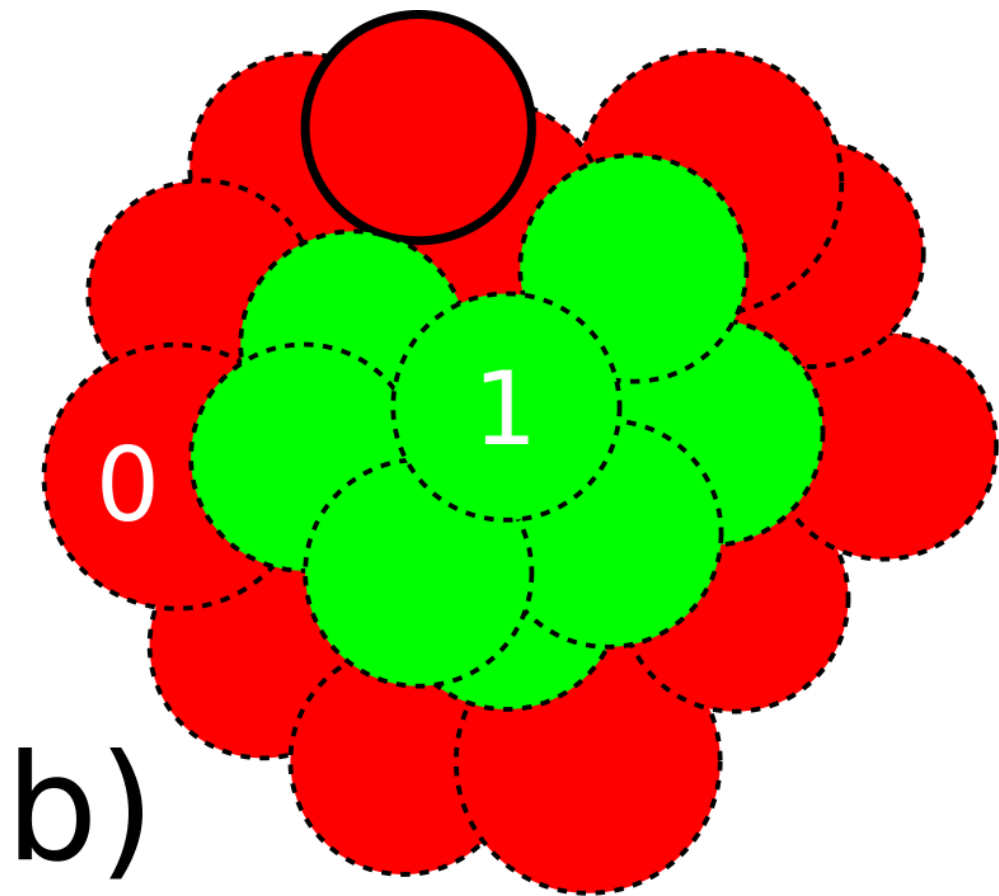
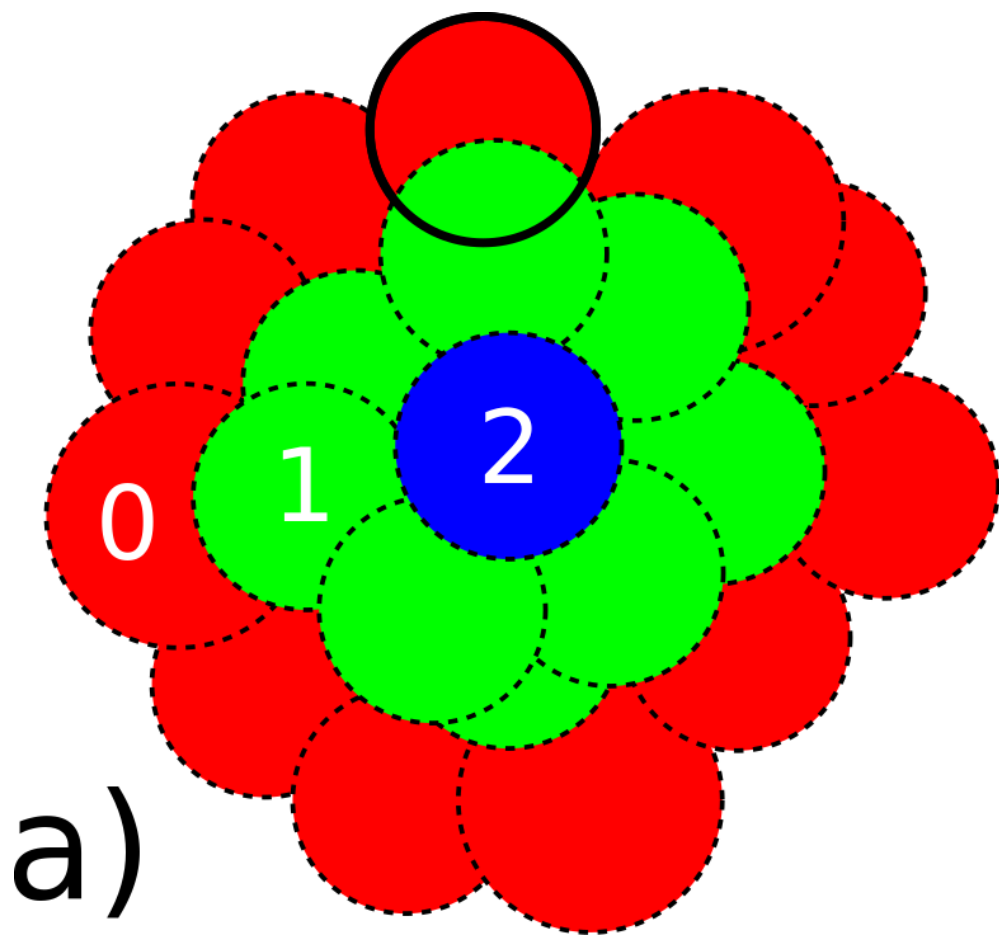
Internal Cool Down

Surface Hot Down

Internal Cool Up

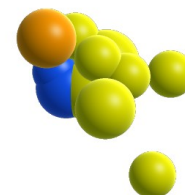
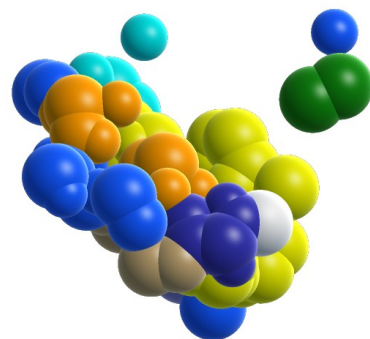
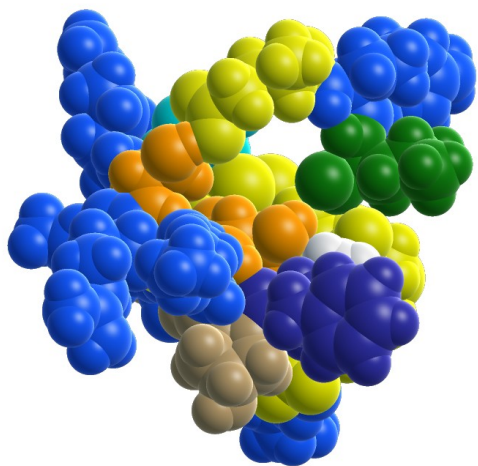
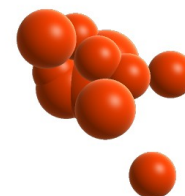
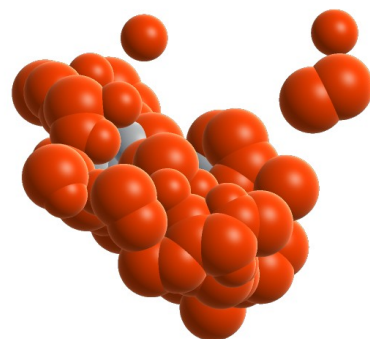
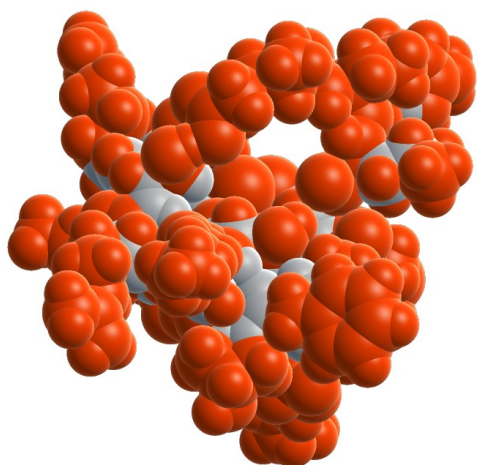
Cold Hot

Layers



Layers

Results



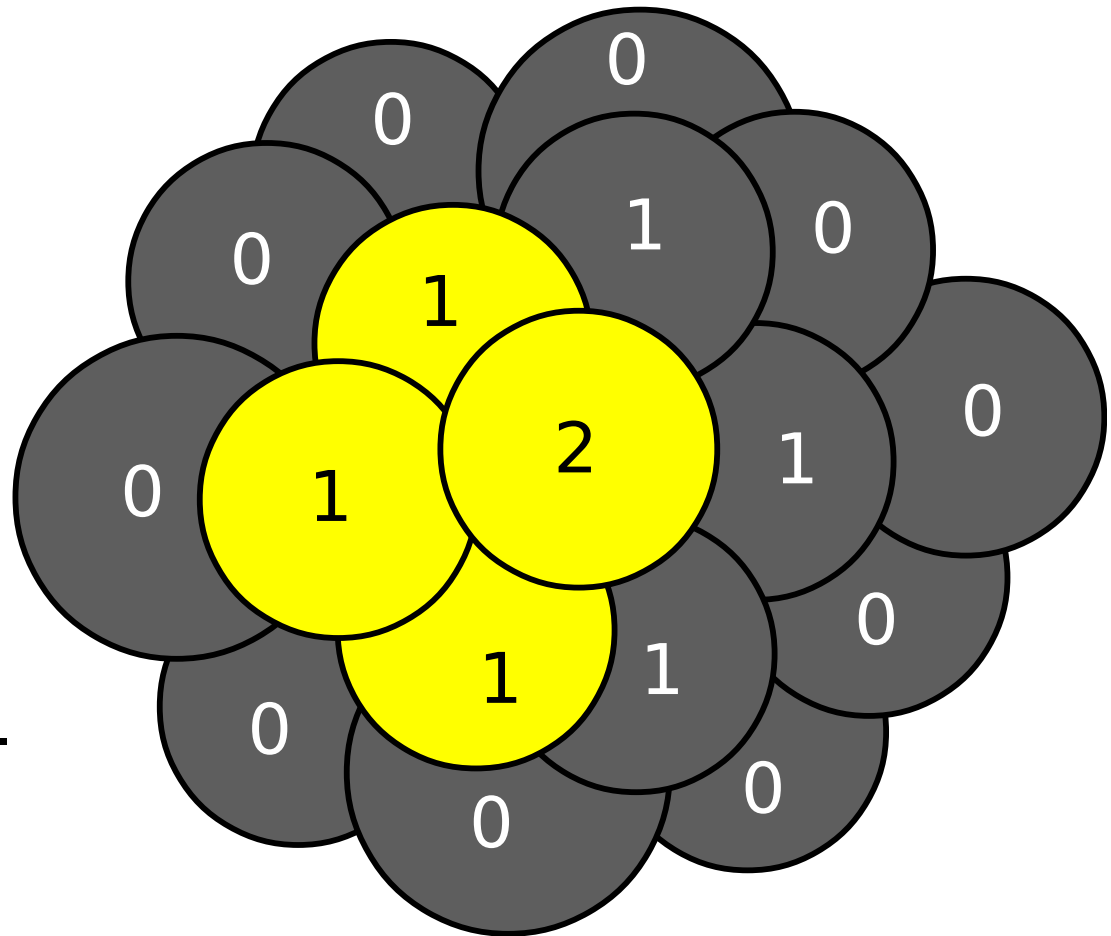
Layer 0

Layer 1

Layer 2

Residue Surface-Proximity

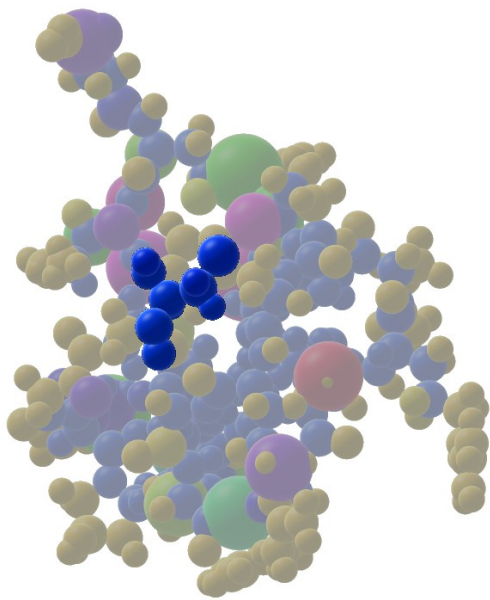
- Proteins consist of amino acid residues
- Scientists are interested in their movement
- Average layer membership over folding simulation tracked
- **Surface-proximity** or **core-proximity** per amino acid computed



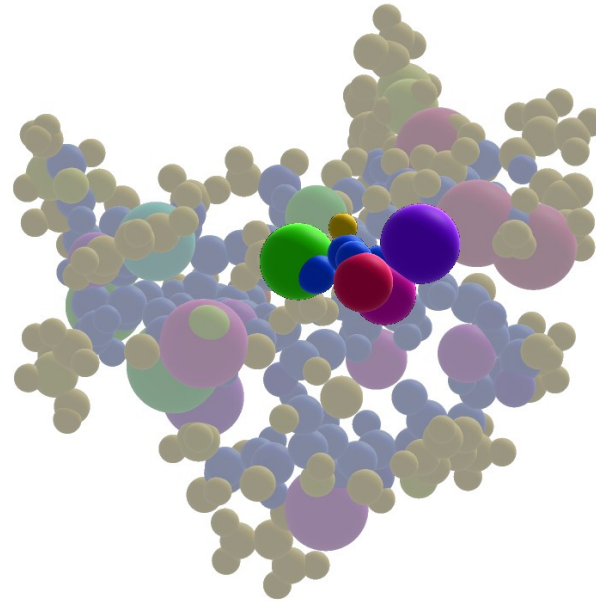
Evaluation

Evaluation

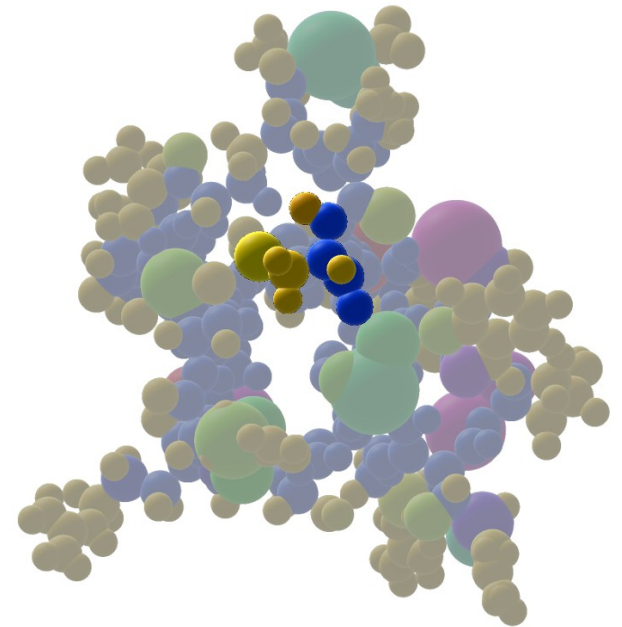
Ascension



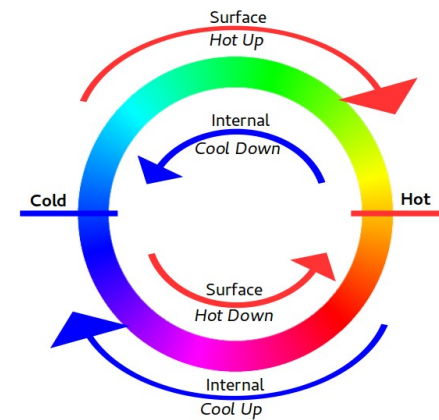
~ 9.4 ns



~13 ns

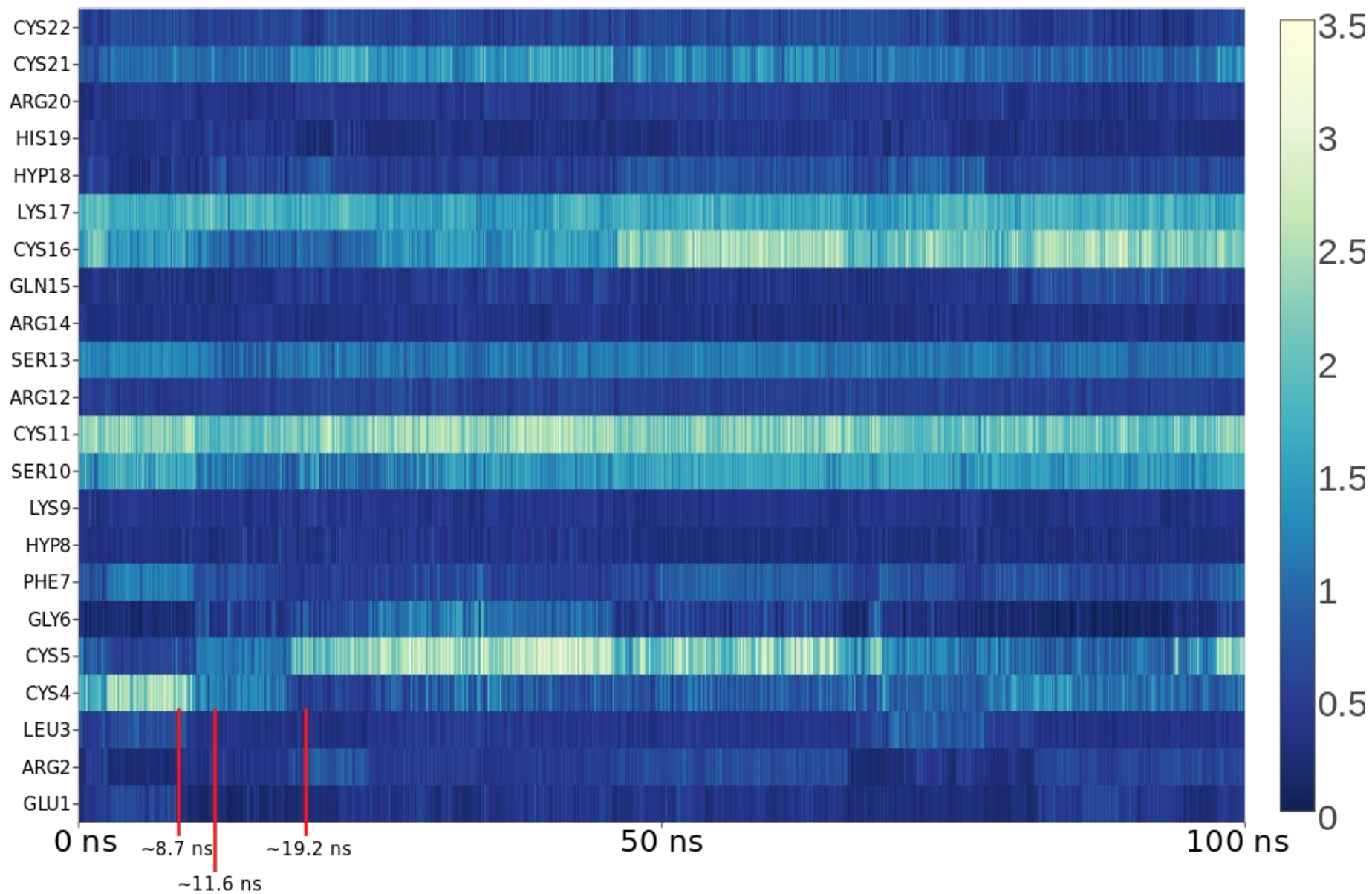


~ 20.5 ns



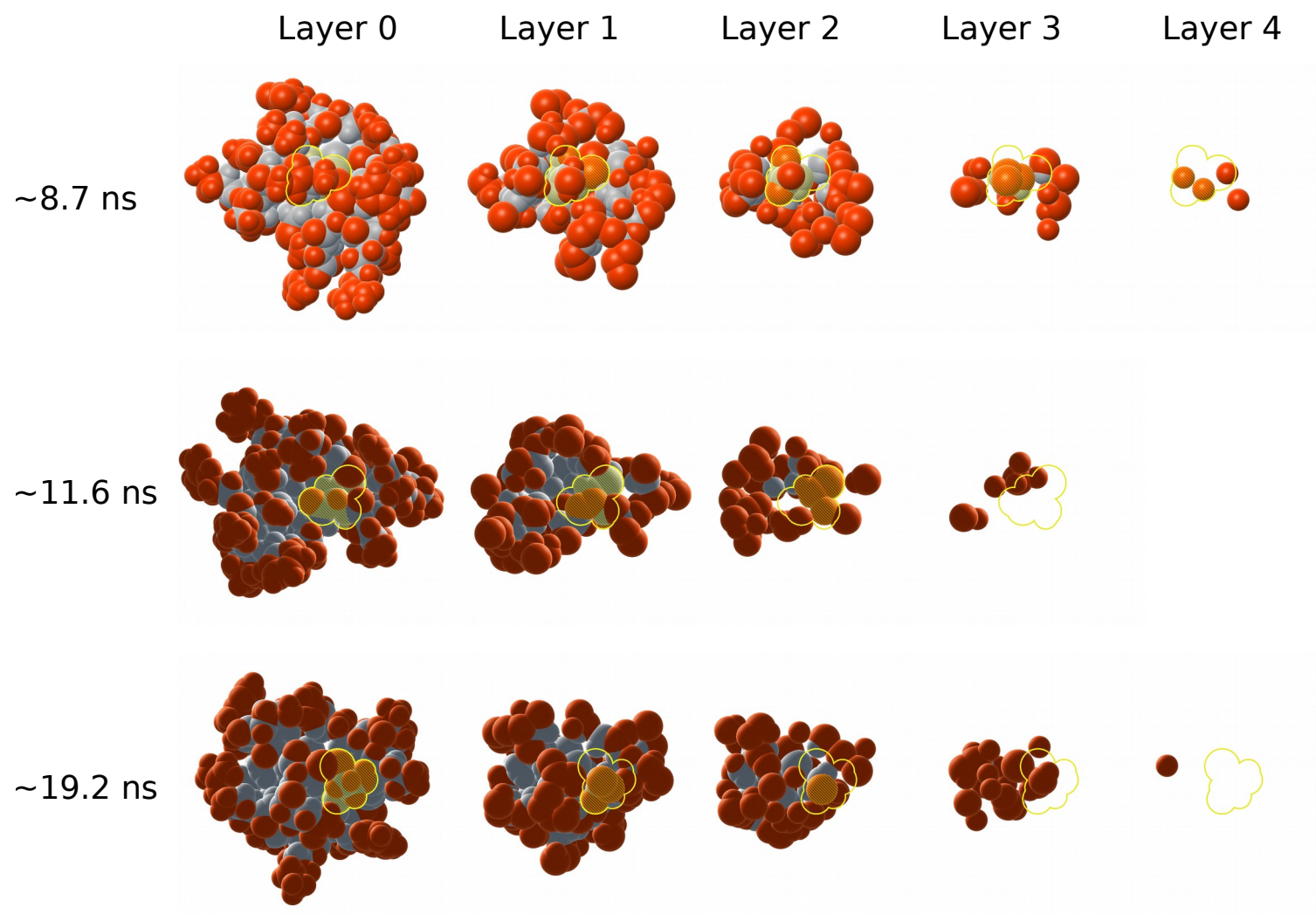
Evaluation

Residue Surface-Proximity



Evaluation

Residue Surface-Proximity



Conclusion

- Supports scientists in molecule design
- Surface dynamics visualization and analysis is novel research area
- Interdisciplinary field with potential

Thank you for your attention!