VU Visualisierung 2 (186.833)

Rendering molecules for fun and profit

Implementation

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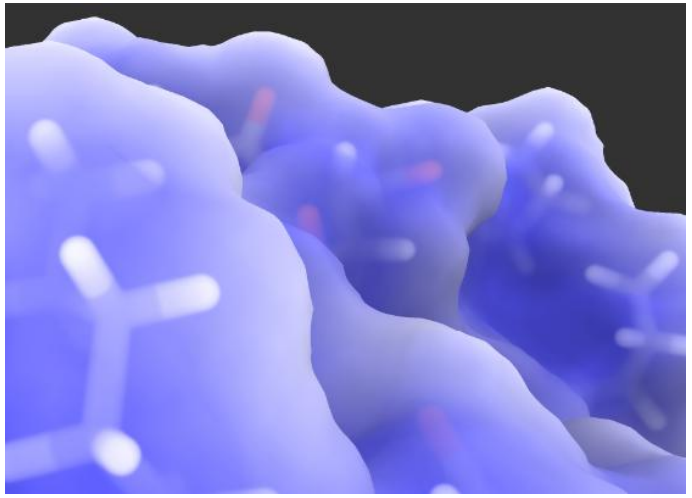
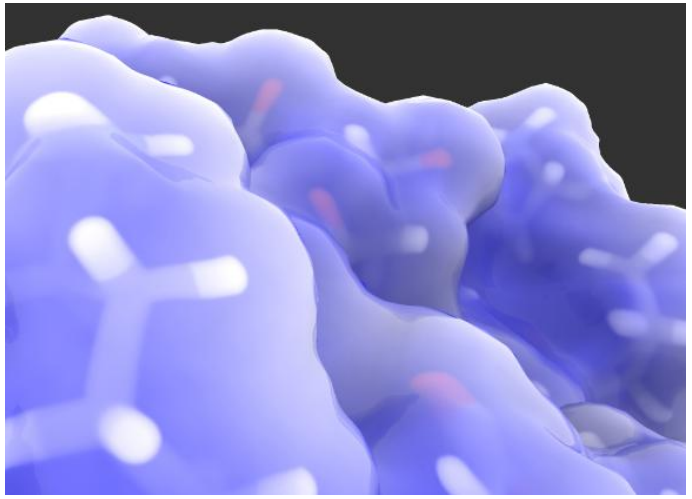
Short Article Summary

- Displaying molecules is hard
- Traditional methods inaccurate
- Better visibility with
  - Subsurface scattering
  - Reflections and refractions
  - Transparency of internal structure



Visualization without reflections and refractions



Visualization with reflections and refractions

Concept

- Rasterization of internal structure (sticks)
- Surface rendering with raymarching
- Apply effects
  - 1. Transparency + translucency
  - 2. Subsurface scattering
  - 3. Transparent structures beneath the surface
  - 4. Reflections and refractions

Implementation & Data

- WebGPU
  - Compute shader
  - Classic mesh rasterization
  - Raymarching
- Typescript
- SvelteKit
- RCSB PDB

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P. Hermosilla and S. Maisch and P.-P. Vázquez and T. Ropinski

Improving Perception of Molecular Surface Visualizations

Eurographics Workshop on Visual Computing for Biology and Medicine, 2018