



VU Visualisierung 2 (186.833)

Rendering molecules for fun and profit

Final Presentation

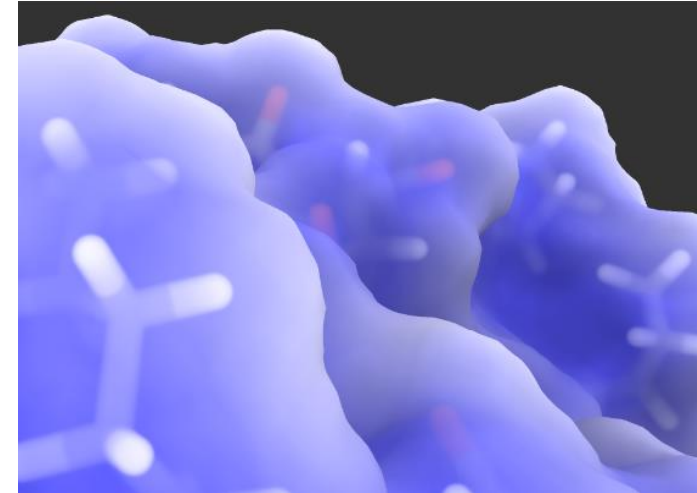
Yannic Ellhotka & Simon Wesp

11776184 & 11709457

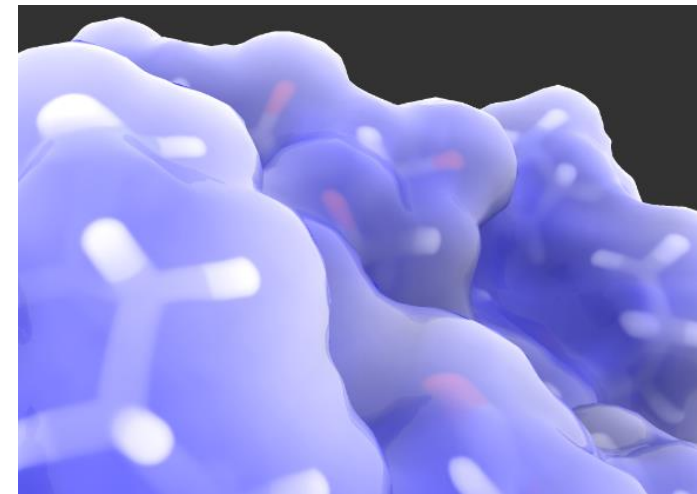
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- Displaying molecules is hard
- Traditional methods inaccurate
- Better visibility with
 - Subsurface scattering
 - Reflections and refractions
 - Transparency of internal structure



Visualization without reflections and refractions



Visualization with reflections and refractions



- Rasterization of internal structure (balls and sticks)
 - Geometry
 - Instancing
- Surface rendering with ray marching
 - Signed distance field calculated with a compute shader
- Apply effects
 - 1. Transparency
 - 2. Subsurface scattering
 - 3. Reflections



- WebGPU
- Typescript
- SvelteKit
- RCSB PDB



- 2 Render Passes + Blending
 - Rasterization
 - Ray marching
- Mini WebGPU Framework



- WebGPU support and implementation varies a lot
- Debugging shaders
- Optimization - rendering 100k+ objects
- Memory layout & management
- Protein files invalid



Demo :)



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

