VU Visualisierung 2 (186.833)

Rendering molecules for fun and profit

Final Presentation

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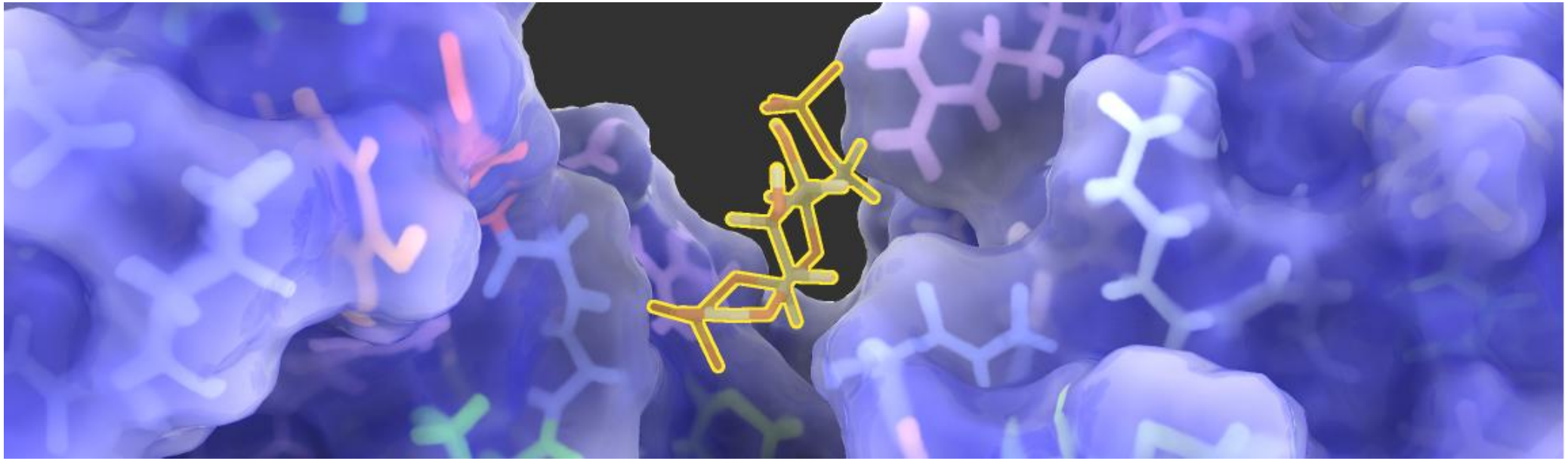
Rendering molecules for fun and profit

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

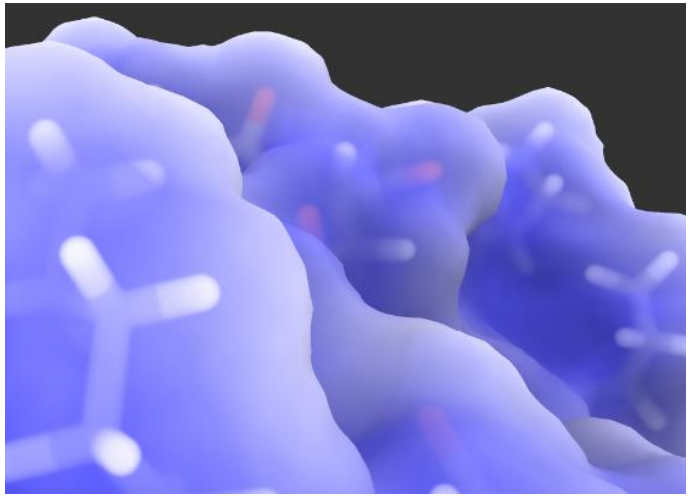
Improving Perception of Molecular Surface Visualizations

Eurographics Workshop on Visual Computing for Biology and Medicine, 2018

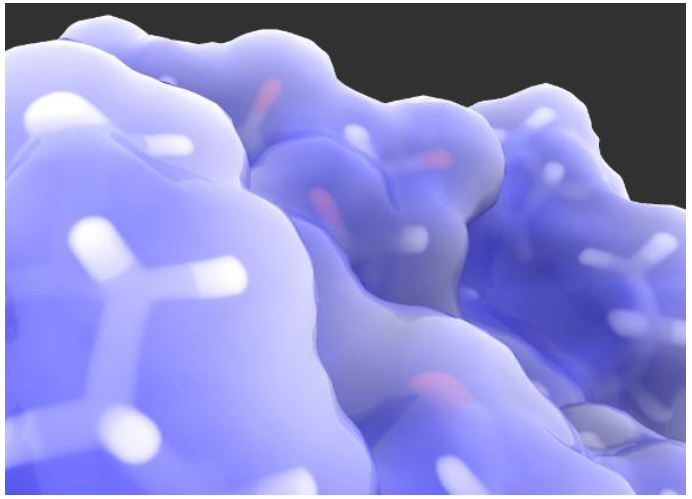


Short Article Summary

- 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

Implementation

- 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

Implementation & Data

- WebGPU
- Typescript
- SvelteKit
- RCSB PDB

Challenges

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

Demo

Demo :)