

Accelerated Visualization of Transparent Molecular Surfaces in Molecular Dynamics

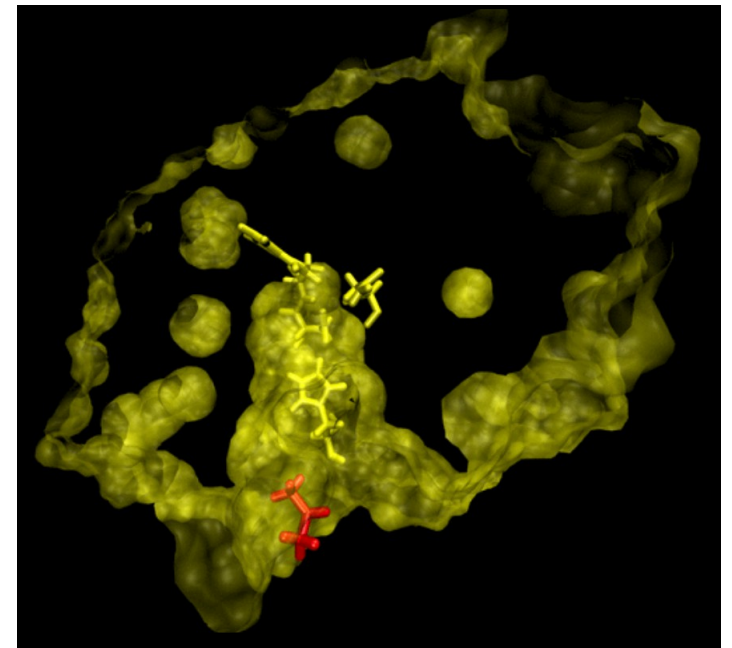
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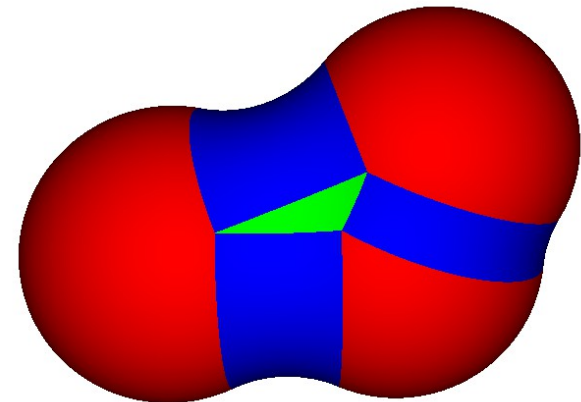
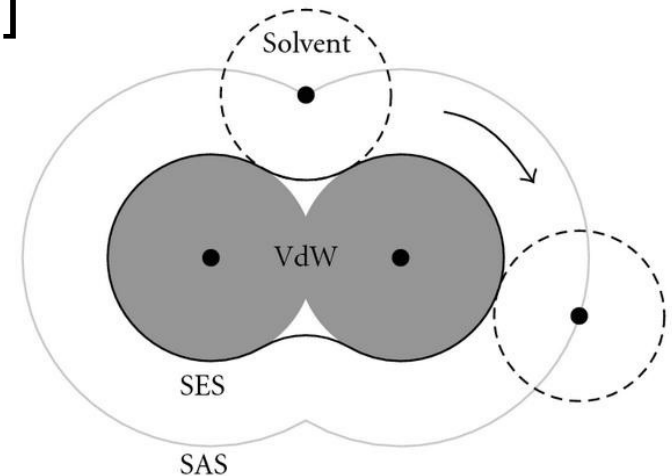
Protein Surfaces in Biochemistry

- Proteins – in all living cells
- Protein features – delimited by surfaces
 - Molecular surface – pockets
 - Transport pathways – tunnels
 - Closed voids – cavities
- Molecular Dynamics
 - Simulation of natural motion
 - Surfaces **change**



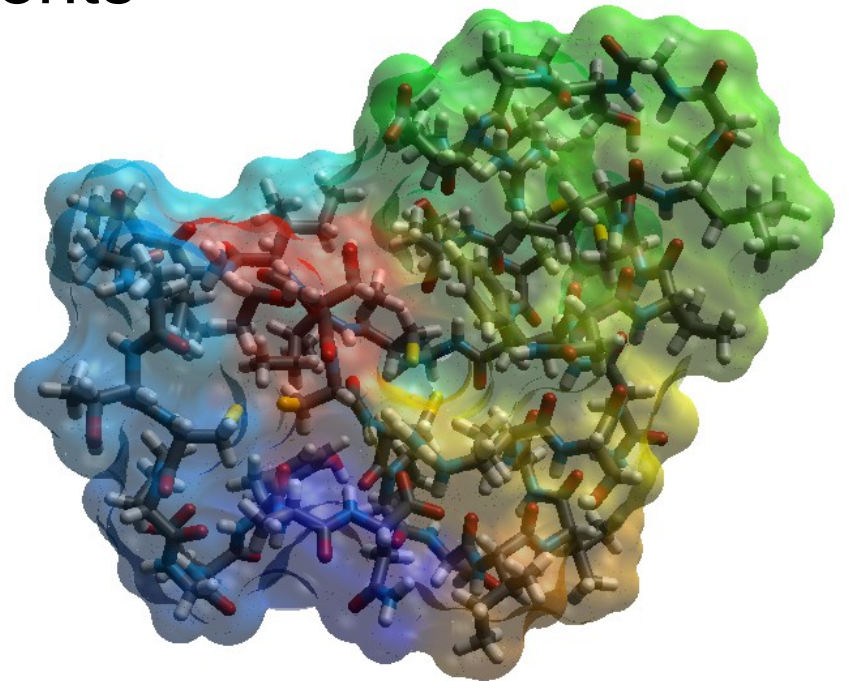
Molecular Surface

- Solvent Accessible [Lee et al. '71]
 - Spherical patches
- Solvent Excluded [Connolly '83]
 - Spherical patches
 - Toroidal patches
 - Spherical triangles
 - reentrant



Transparent Molecular Surface

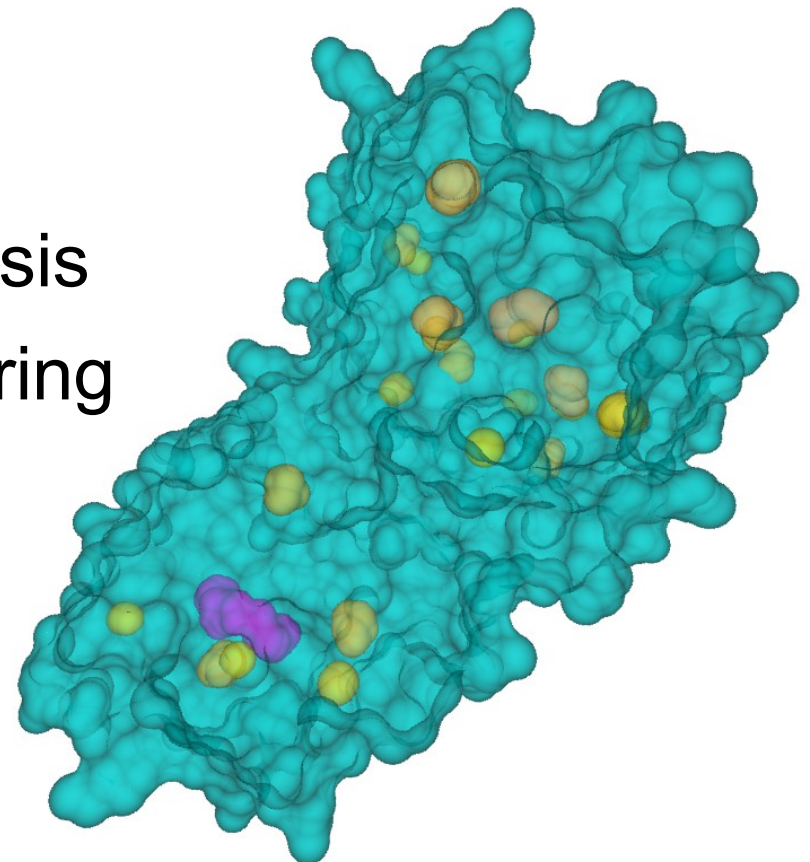
- Molecular surface using OIT [Kauker et al. '13]
 - Fragments of all atom spheres
 - CSG operations on fragments
 - **Correct** transparency
 - **High** depth complexity
 - 188 layers/10000 atoms



Our Accelerated Method

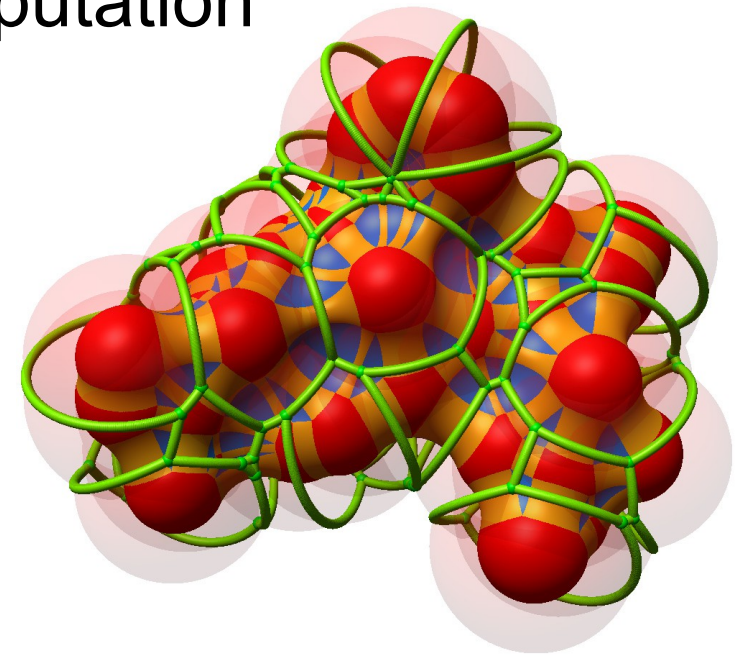
Idea: Compute and render only surface

- Method overview:
 - 1) Surface computation
 - 2) Surface components analysis
 - 3) Transparent surface rendering
- Visual enhancements:
 - Cavity coloring by area
 - Opacity modulation



Step 1: Surface Computation

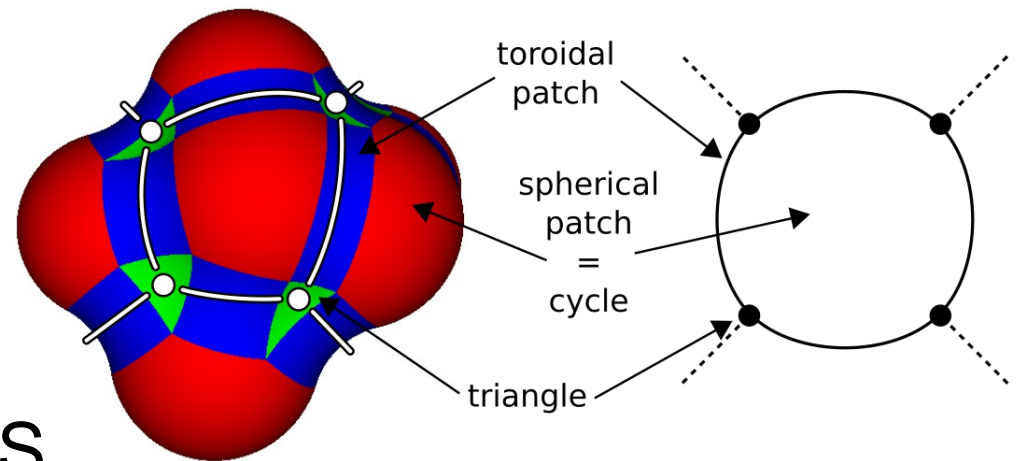
- Contour-buildup algorithm [Totrov et al. '96]
 - Accelerated and **localized** computation
- Parallelization
 - Multiple CPUs [Lindow et al. '10]
 - Single GPU [Krone et al. '11]
- Rendering using transparency
 - Cavities – possible occlusion



Step 2: Surface Analysis

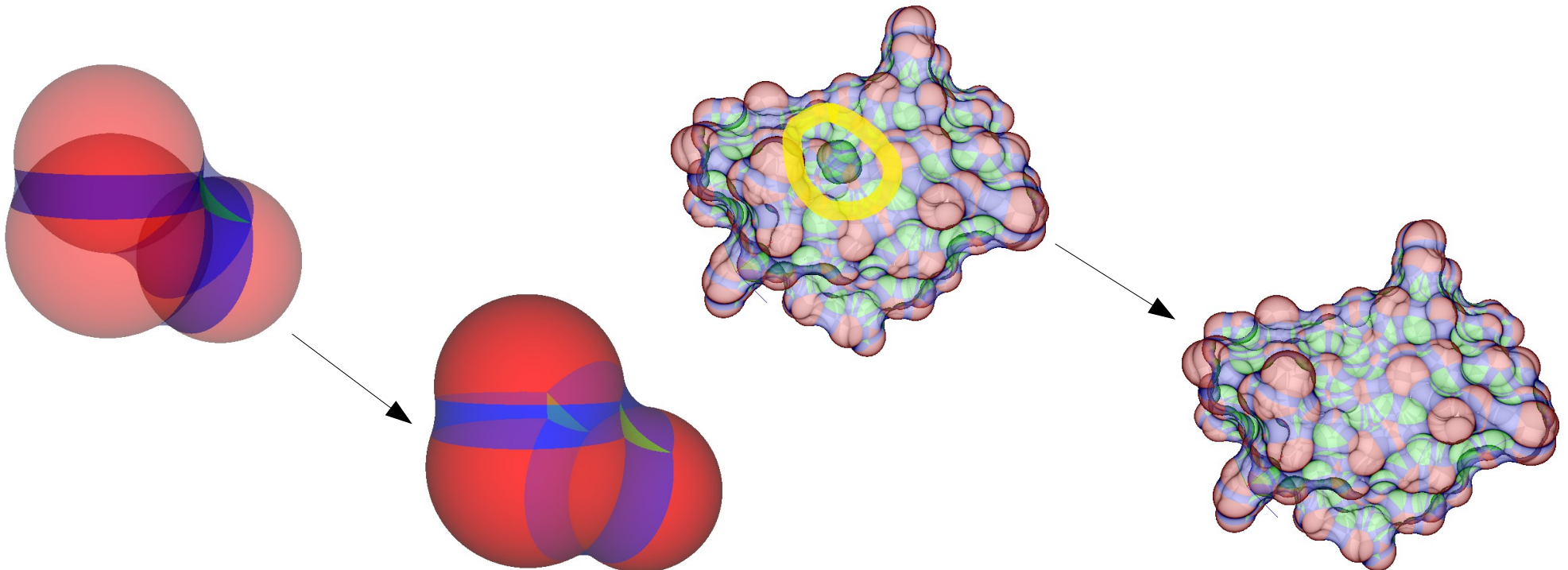
- Ideas:
 - Surfaces = isolated connected components (CC)
 - Spherical patches are enclosed with tori
 - Tori connect triangles

- Algorithm:
 - 1) Adjacency list
 - 2) CC analysis – use BFS
 - 3) Cycles forming patches



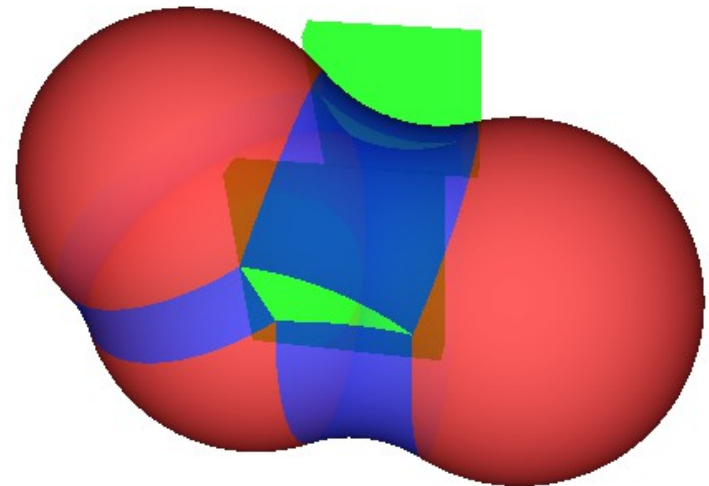
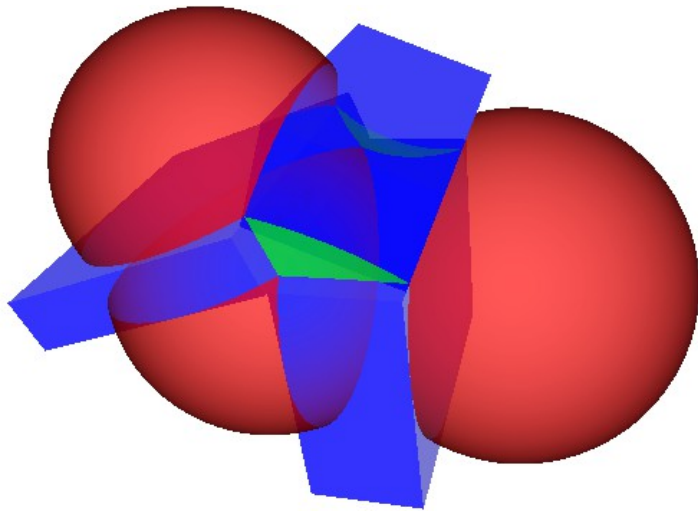
Step 3: Surface rendering I

- Surface graph benefits:
 - Extraction of **all** SES patches
 - Extraction of inner cavities



Step 3: Surface rendering II

- Ray-casting
 - Improved performance of ray-casting individual SES patches using OBBs



Results I

- Transparent SES visualization:
 - Static and dynamic structures – PDB ID
 - SES probe size = 1,4 Å

Results II

- Performance comparison
 - Resolution: 1024 x 768
 - GPU: NVIDIA GF GTX 680

		Our method		Kauker et al.		
PDB ID	Atoms	DL	FPS	DL	FPS	Speedup
1OGZ	~650	12	48.1	117	31.0	1.55
1VIS	~2500	15	34.1	135	11.2	3.04
4ADJ	~10000	19	15.5	188	6.2	2.50

Summary

- Contribution
 - Accelerated transparent dynamic SES visualization
 - Improved memory efficiency
- Limitations
 - Uneasy to perceive transparency in still images
 - Unable to detect open pathways – tunnels
- Future work
 - Detection and coloring of tunnels
 - (Employment of efficient BFS algorithm)

Thank you for your attention!