Accelerated Visualization of Transparent Molecular Surfaces in Molecular Dynamics

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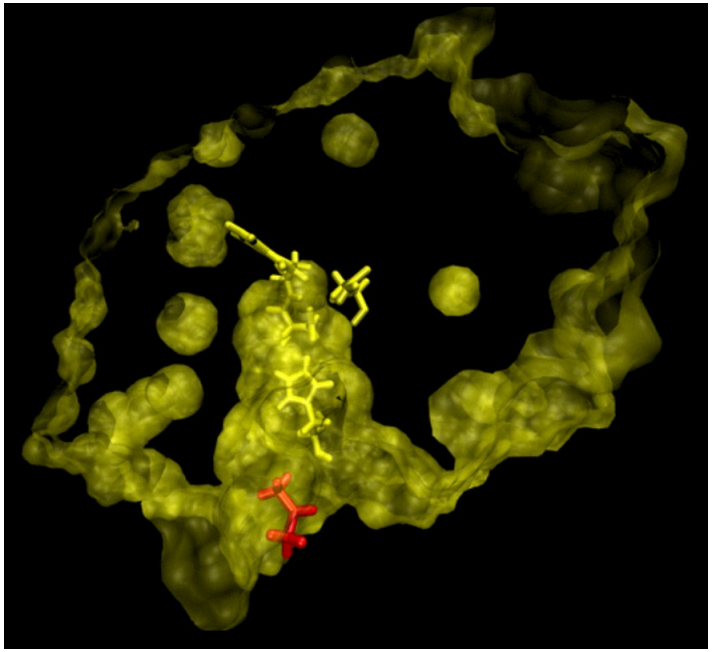
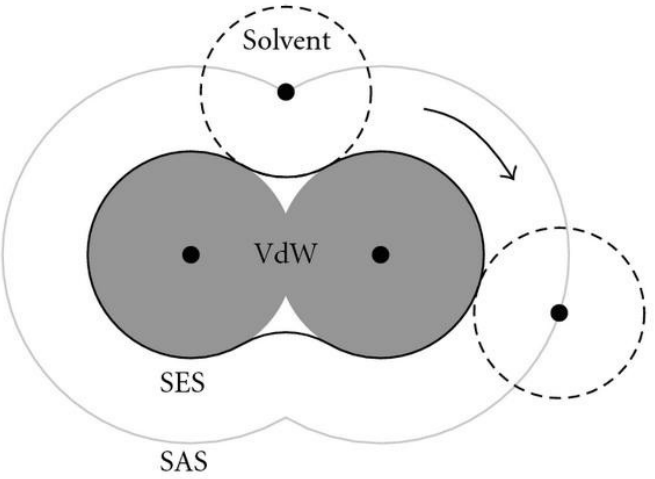
Protein Surfaces in Biochemistry

- 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**

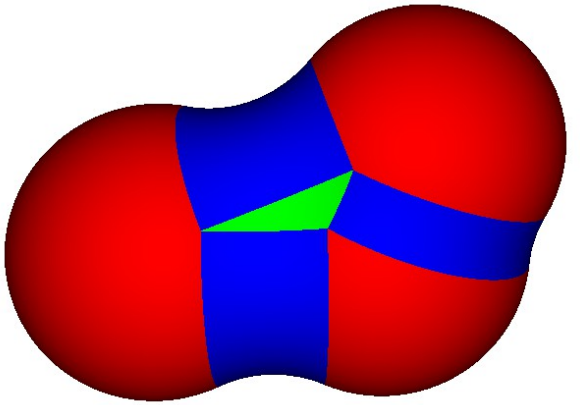


Molecular Surface

- Solvent Accessible [Lee et al. '71]
  - Spherical patches

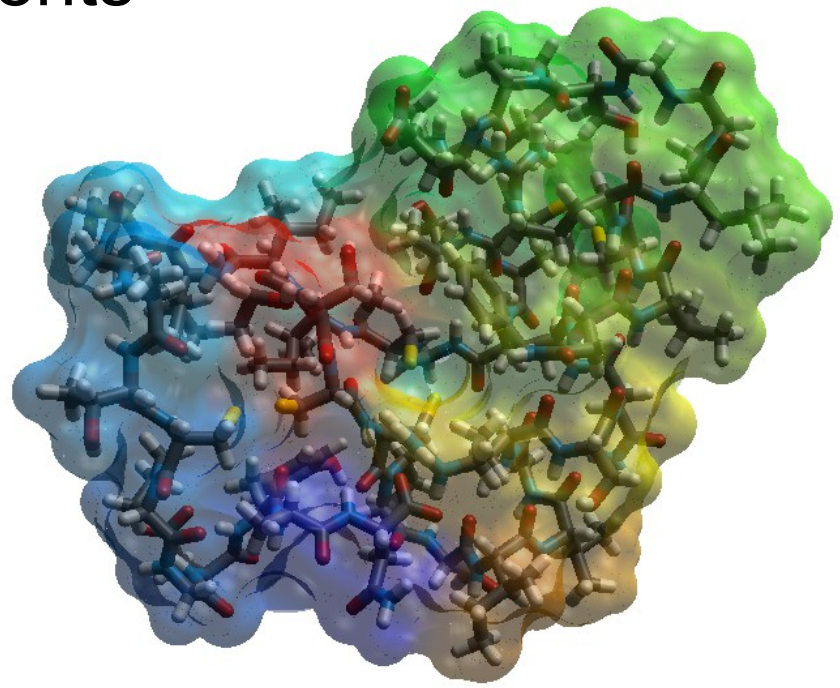


- Solvent Excluded [Connolly '83]
  - Spherical patches
  - Toroidal patches
  - Spherical triangles
    - reentrant



Transparent Molecular Surface

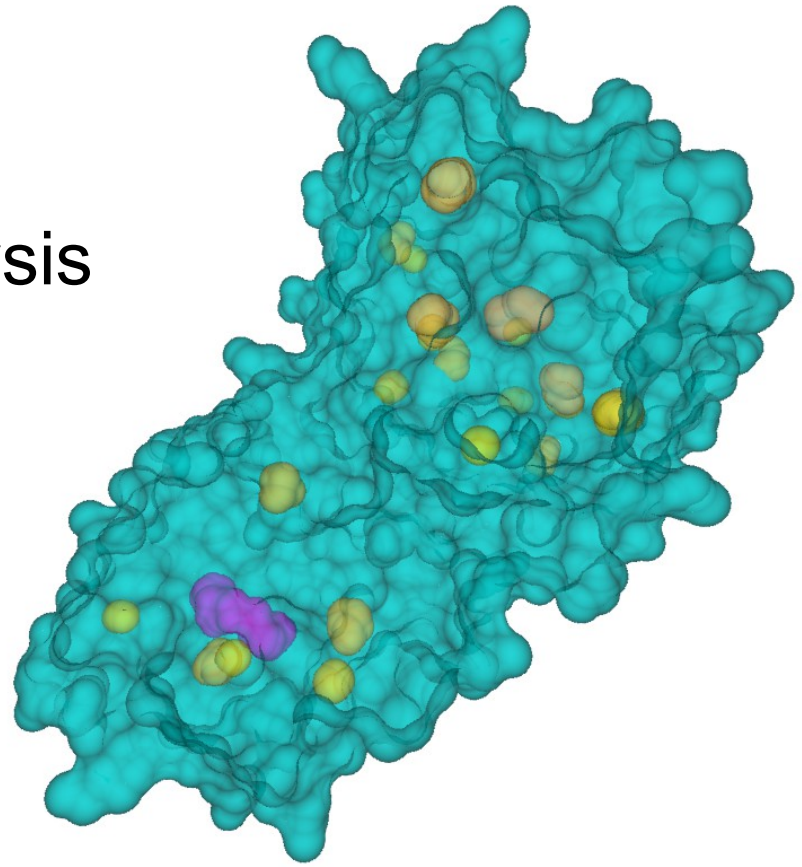
- Molecular surface using OIT [Kauker et al. '13]
  - Fragments of all atom spheres
  - CSG operations on fragments
  - **Correct** transparency
  - **High** depth complexity
    - 188 layers/10000 atoms



Our Accelerated Method

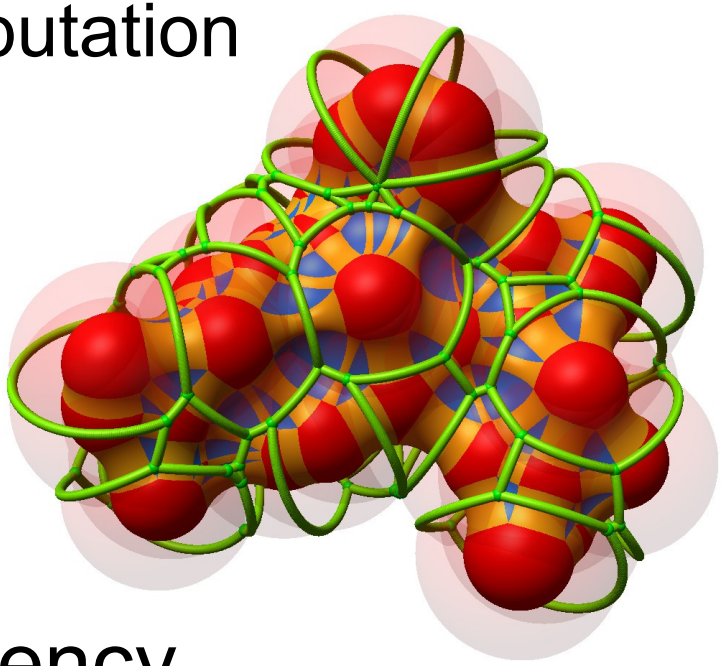
Idea: Compute and render only surface

- Method overview:
  1) Parallel SES computation
  2) Surface components analysis
  3) SES patches ray-casting
- Visual enhancements:
  - Cavity coloring by area
  - Opacity modulation



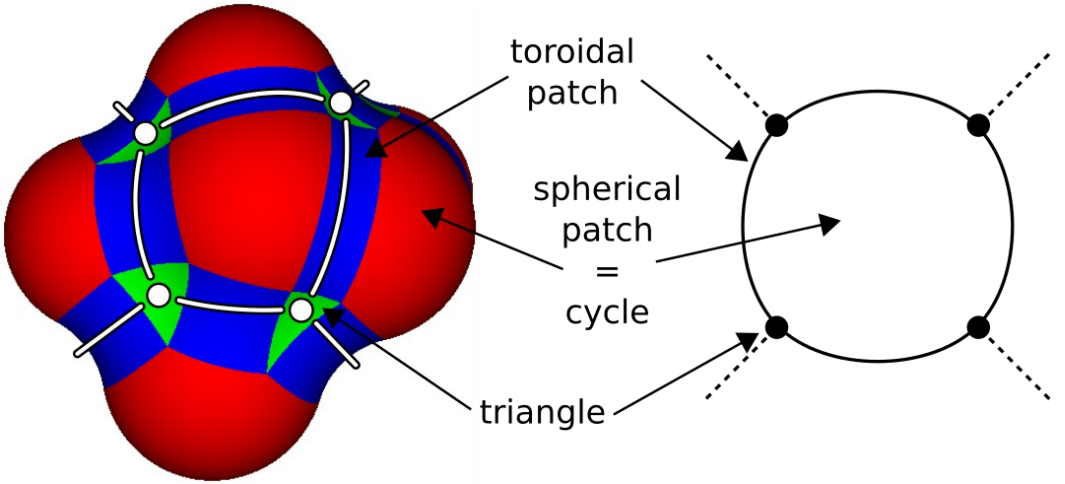
Contour-Buildup Algorithm

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



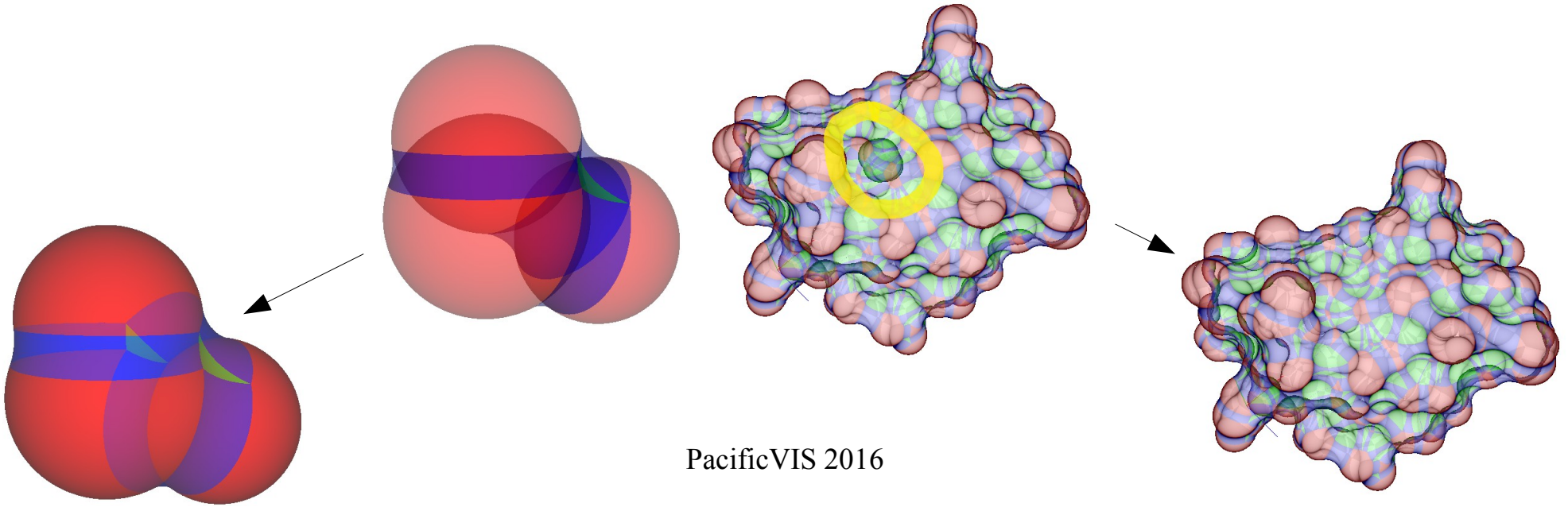
Surface Graph

- Ideas:
  - Surfaces = isolated connected components (CC)
  - Spherical patches are enclosed with tori
  - Tori connect triangles
- Algorithm:
  1) Build adjacency list
  2) Find CCs – use BFS
  3) Find circles for patches



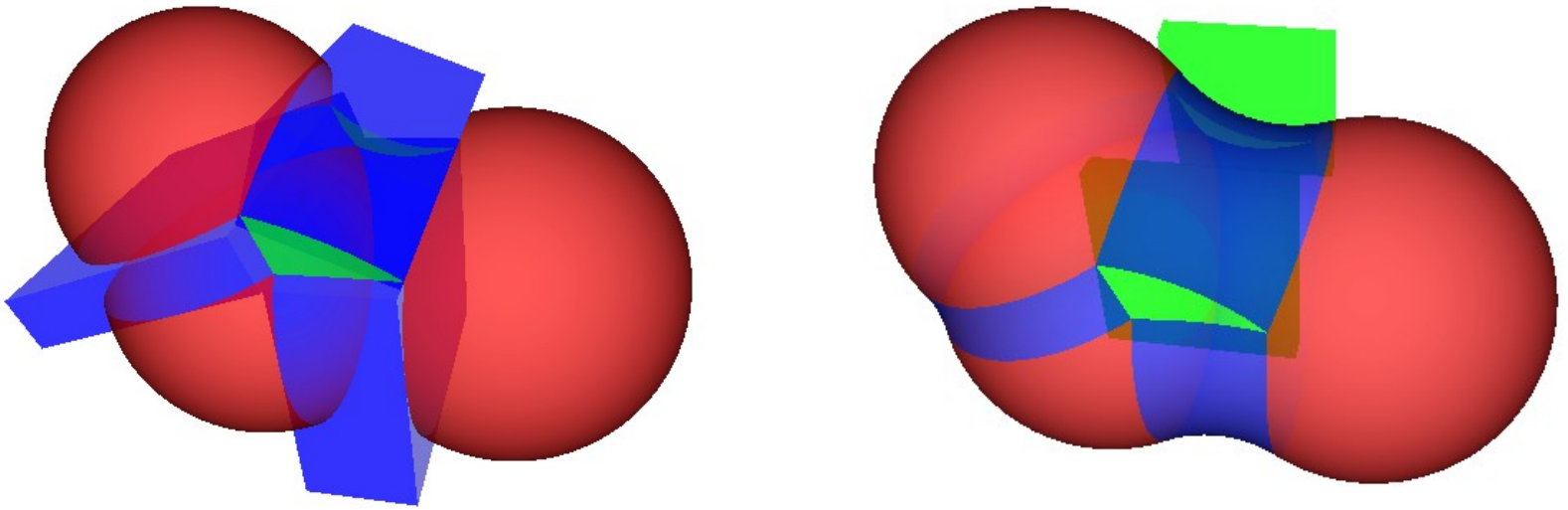
Extended GPU Contour-Buildup I

- Surface graph
  - Extraction of all SES patches
  - Extraction of inner cavities
  - Improved memory efficiency – contour arcs are stored in a hash table



Extended GPU Contour-Buildup 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!