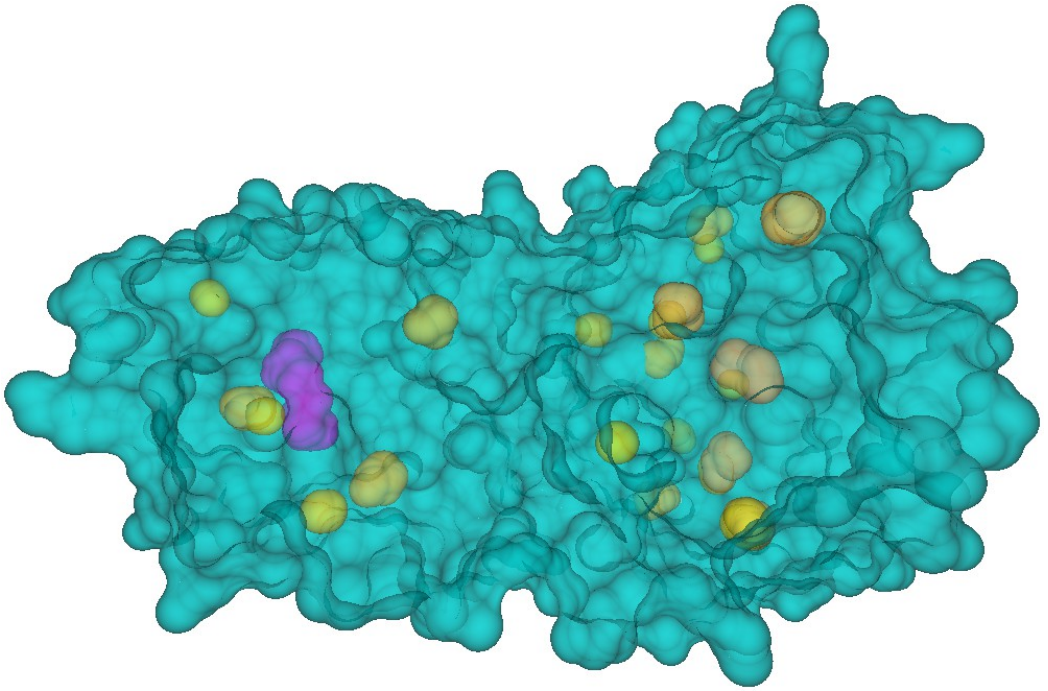

Accelerated Visualization of Transparent Molecular Surfaces in Molecular Dynamics

Adam Jurcik, Jiri Sochor, Barbora Kozlikova (Masaryk Univesity)
Julius Parulek (University of Bergen)

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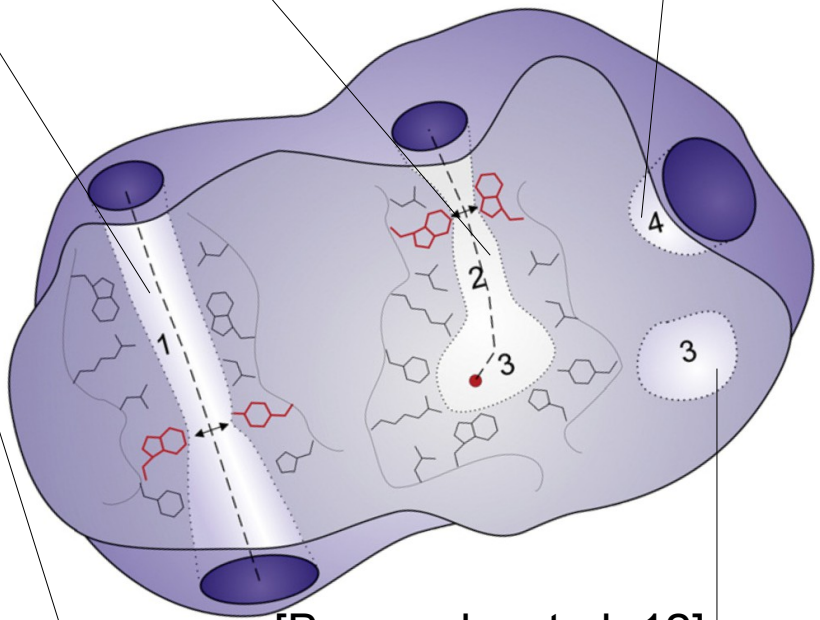
Protein Surfaces in Biochemistry

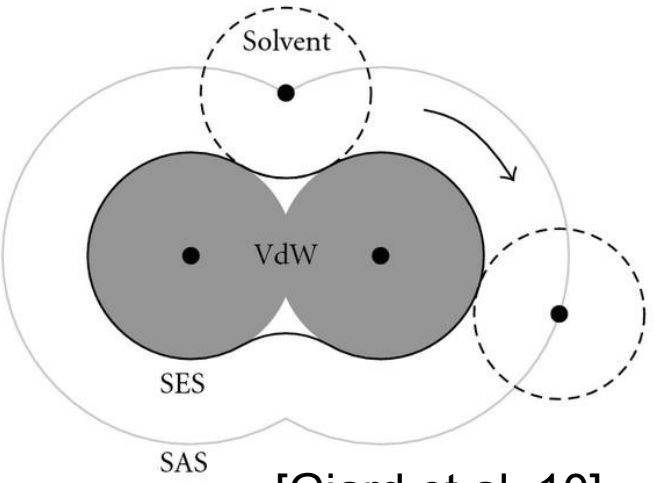
- Proteins – in all living cells
- Protein features – delimited by surfaces
  - Molecular surface – pockets
  - Transport pathways – channels, tunnels
  - **Closed voids – cavities**
- Molecular Dynamics
  - Natural motion simulation
  - Surfaces change



[Brezovsky et al. 12]

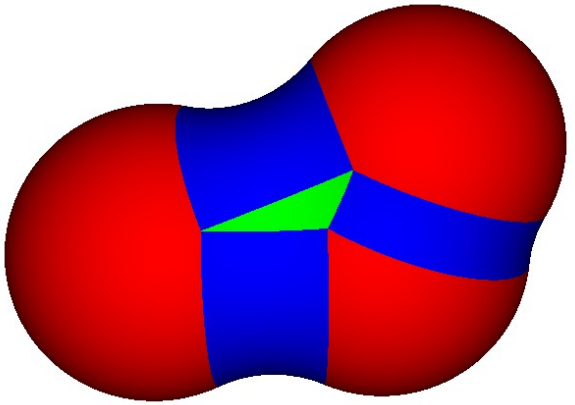
Molecular Surface

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



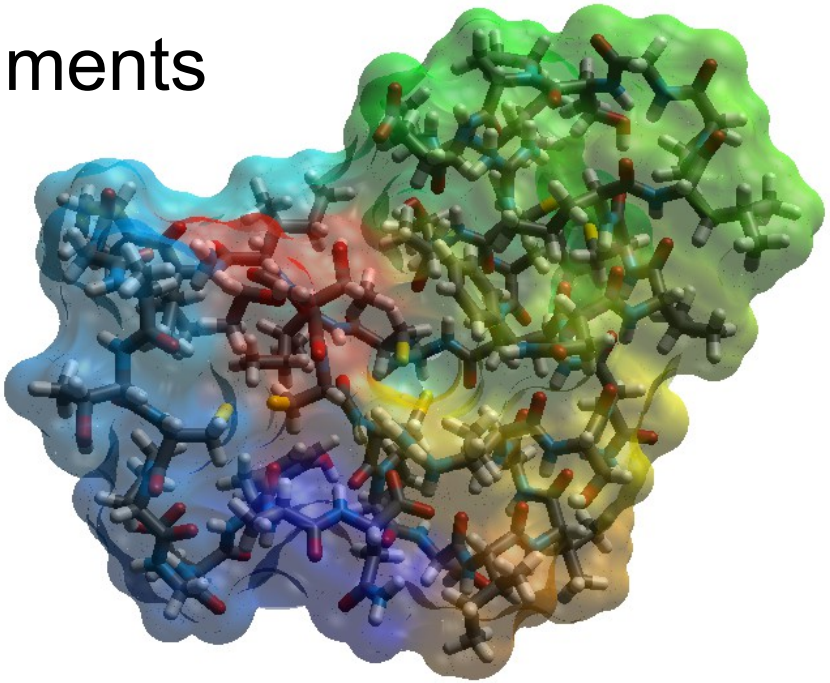
[Giard et al. 10]

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



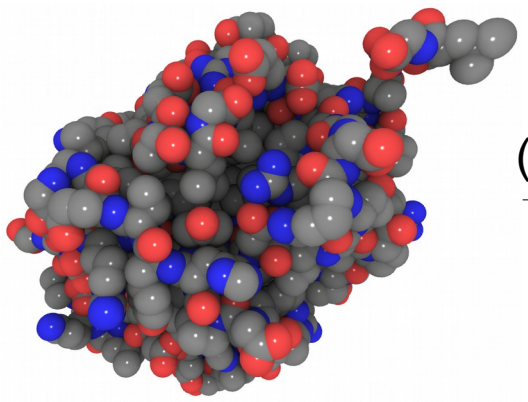
Transparent Molecular Surface

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

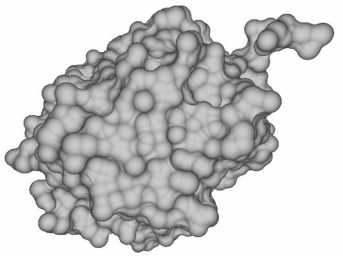


Accelerated Transparent MS

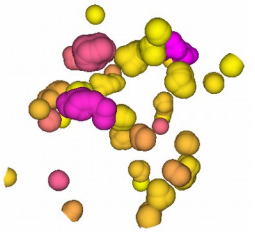
Input: Atom positions



(algebraic) SES

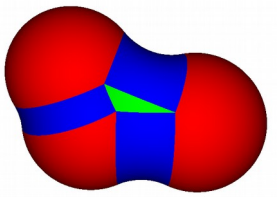


Cavities

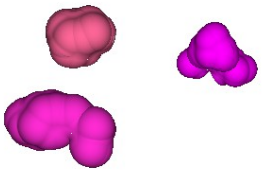


Per frame GPU steps

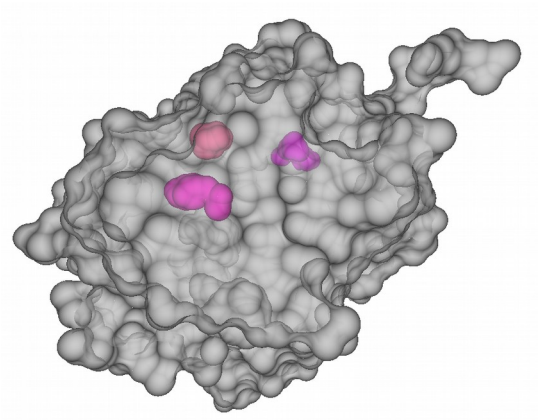
SES patches



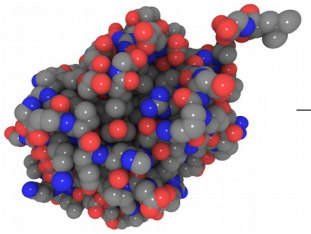
Ray-casting



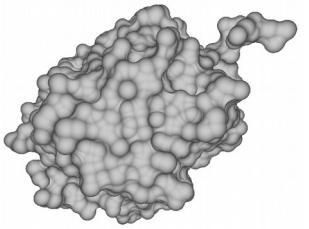
Transparency
(A-buffer)



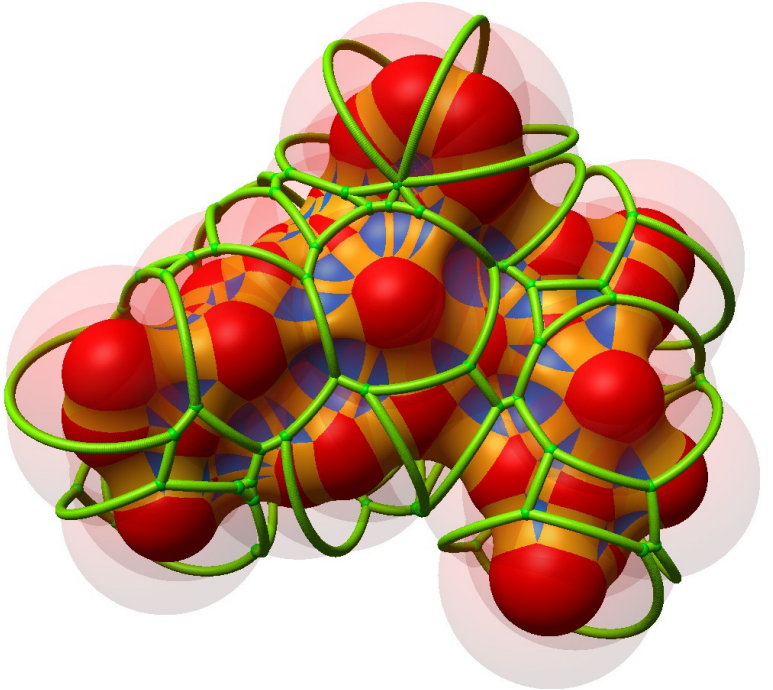
Output: Transparent SES

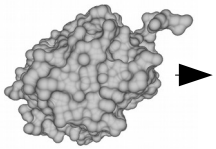


Surface Computation

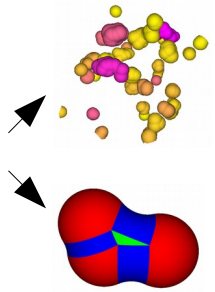


- Contour-buildup algorithm [Totrov et al. '96]
  - Accelerated and **localized** computation
- Parallelization
  - Mutliple CPUs [Lindow et al. '10]
  - Single GPU [Krone et al. '11]

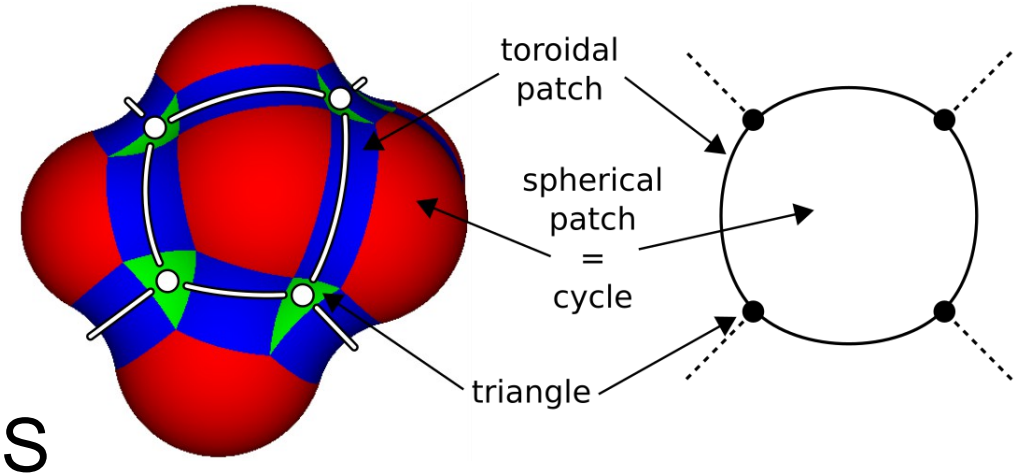




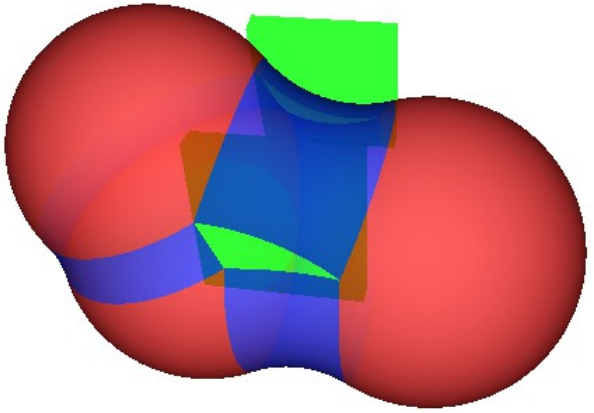
Cavities and patches extraction



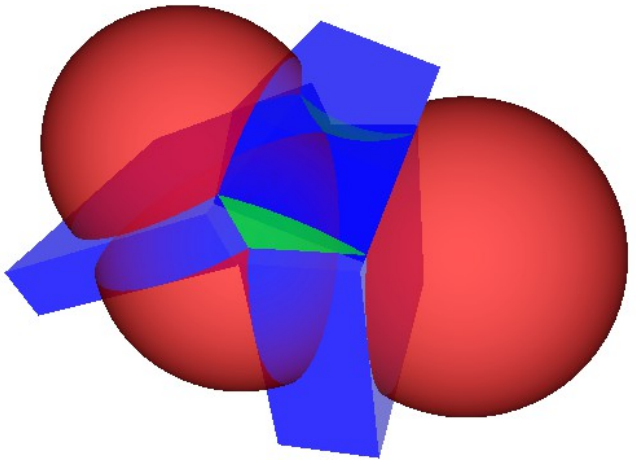
- Observations:
  - Surfaces = isolated connected components (CC)
  - Spherical patches are enclosed with tori
  - Tori connect triangles
- Graph algorithms:
  1) Adjacency list
  2) CC analysis – use BFS
  3) Cycles forming patches



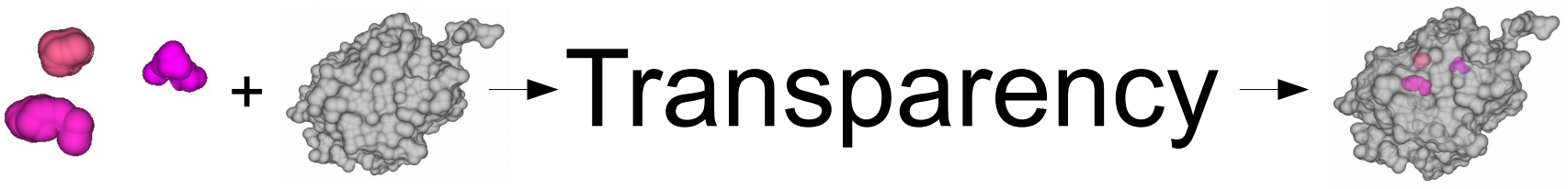
- Individual SES patches
  - OBB splats – geometry shader
  - Less rays – higher performance



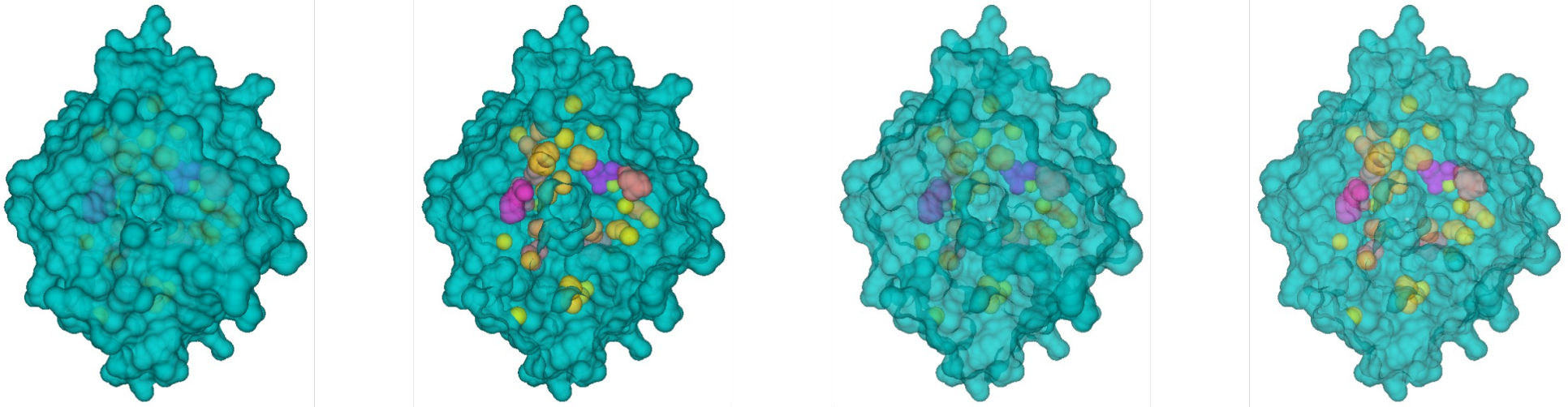
< 8% rays



< 2.5% rays



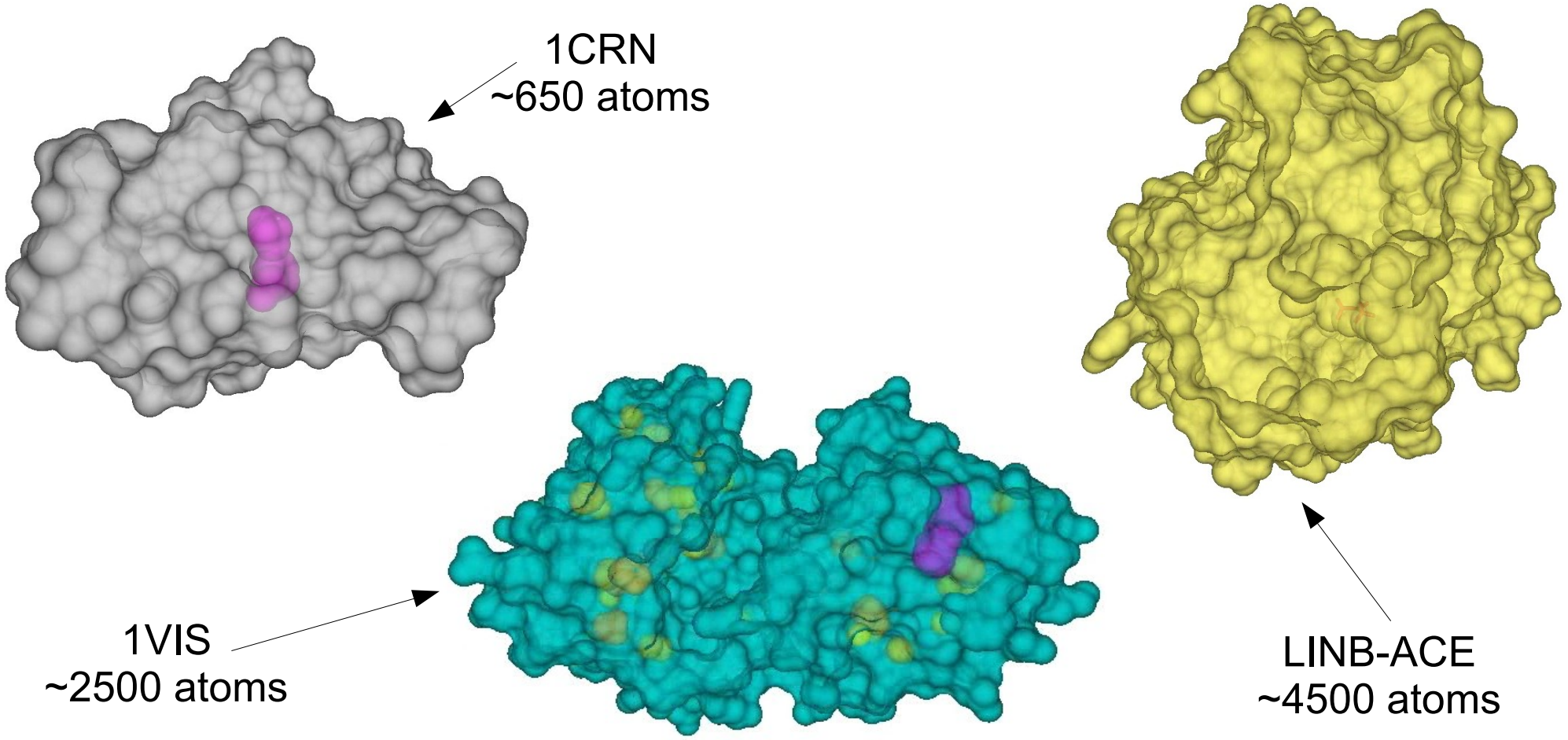
- A-buffer – all surface fragments
- Opacity modulation
  - Overall opacity (O)
  - Entry fragments – opacity suppression (K)



$O = 0.8, K = 1$ $O = 0.8, K = 16$ $O = 0.5, K = 1$ $O = 0.5, K = 16$

Results I

- Transparent SES visualization:
  - Static and dynamic structures – PDB ID



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
  - Interactive transparent dynamic SES visualization
- Limitations
  - Hard to perceive transparency in still images
  - Not detecting open pathways – tunnels
- Future work
  - Detection and coloring of tunnels
  - Experiments with more efficient BFS algorithm

Thank you for your attention!