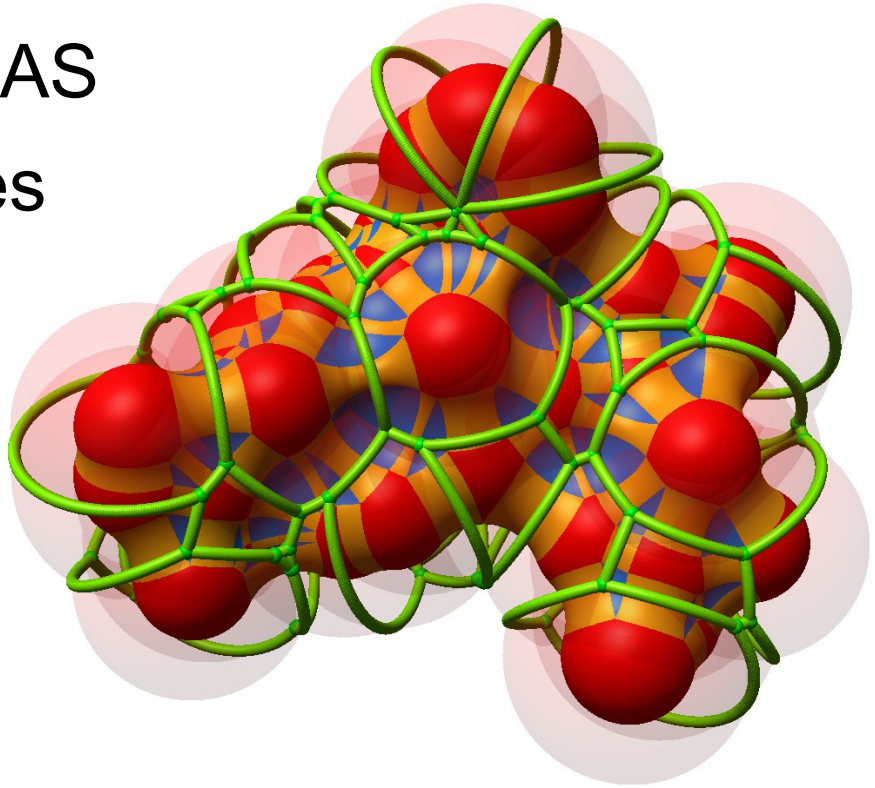
Order-Independent Transparency for Contour-Buildup Algorithm

Contour-Buildup Algorithm

- Totrov et al. (1996) – The contour-buildup algorithm to calculate the analytical molecular surface
  - Calculation of SES/SAS
  - Patches, tori, triangles



Parallelizations of CB

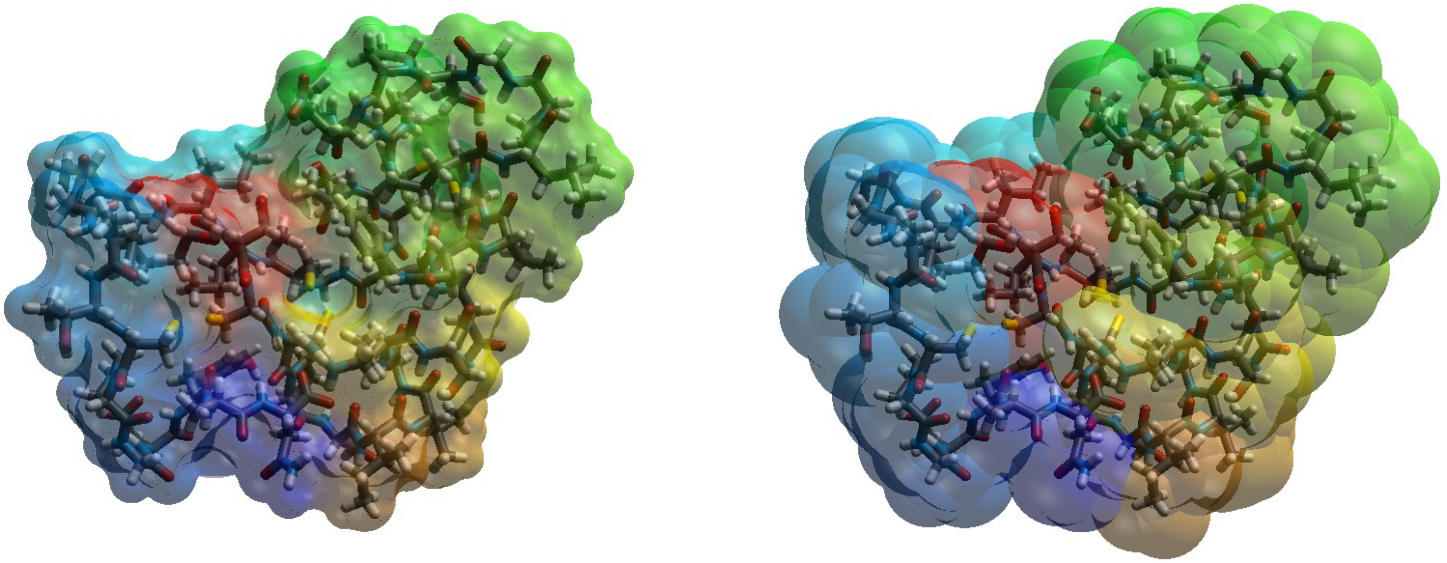
- Lindow et al. (2010) – Accelerated visualization of dynamic molecular surfaces
  - Parallelization on CPUs
  - Implemented in OpenMP
  - GPU ray-casting of surface primitives
- Krone et al. (2011) – Parallel contour-buildup algorithm for the molecular surface
  - Massive parallelization on GPU
  - 9 kernels in CUDA

Order-Independent Transparency

- Depth Peeling
  - Multiple transparent object rendering
  - Peeling layers one by one
  - Dual Depth Peeling – two layers in one pass
- A-buffering
  - All fragments are stored
  - Sorting and composition

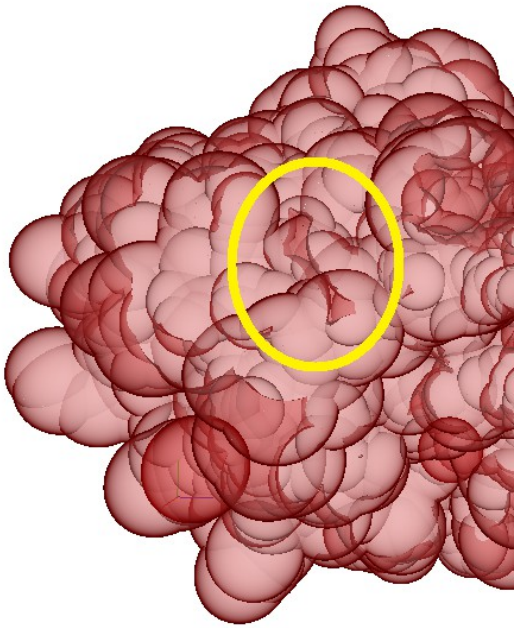
OIT for Molecules

- Kauker et al. (2013) – Rendering molecular surfaces using order-independent transparency
  - Puxels – CSG operations on A-buffer
  - vdW, SES and SAS

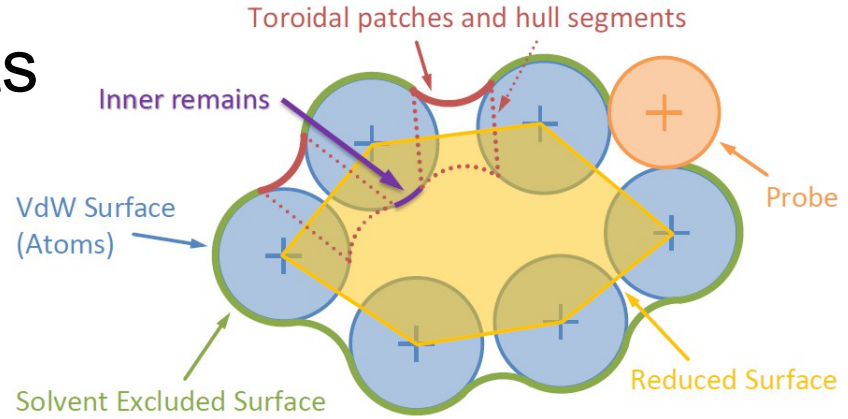


Transparency problems

- Rendering using CB
  - Artifacts – "inner remains"
  - Cavity surface

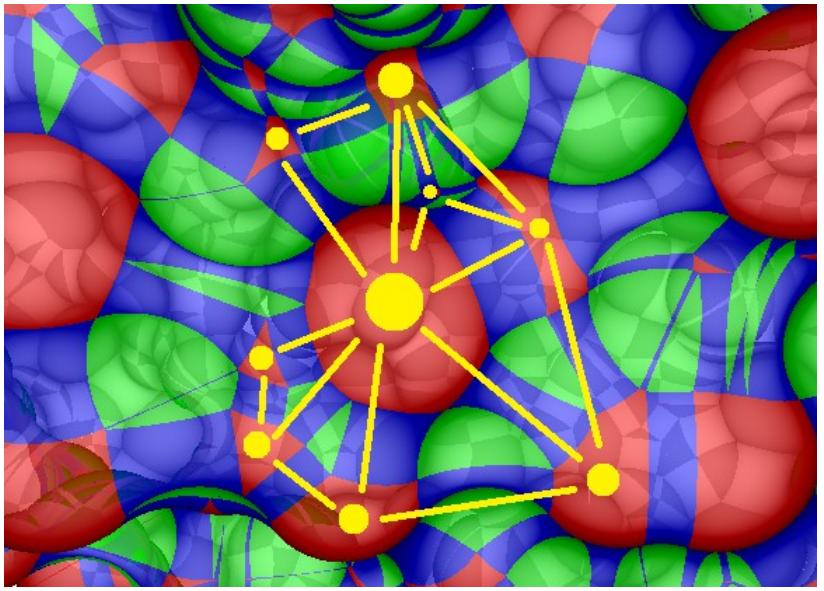


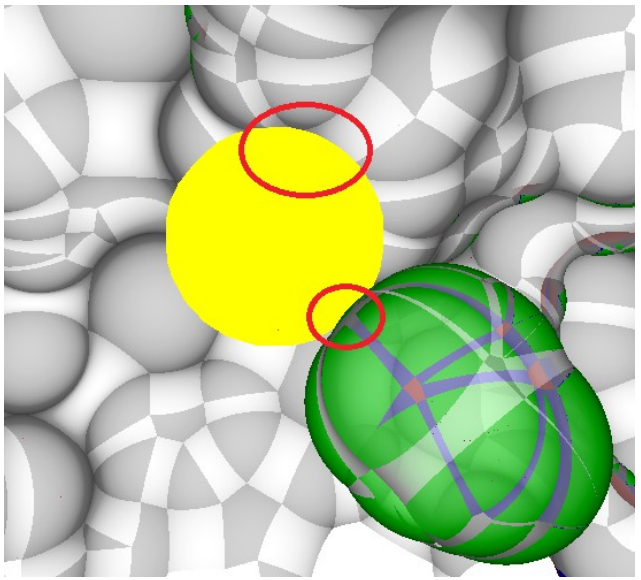
- Rendering with Puxels
  - CSG operations using Reduced Surface
  - Big amount of fragments



Surface Graph I

- Surfaces = isolated connected components:
  1) Spheres connected with tori
     - Easy – already computed during CB
     - Spheres may form multiple surfaces!



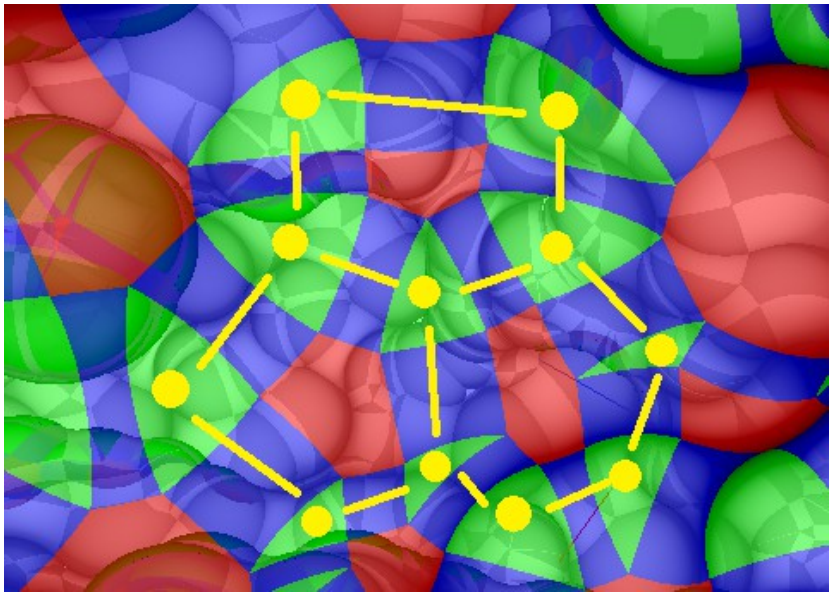


Surface Graph II

- Surfaces = isolated connected components:

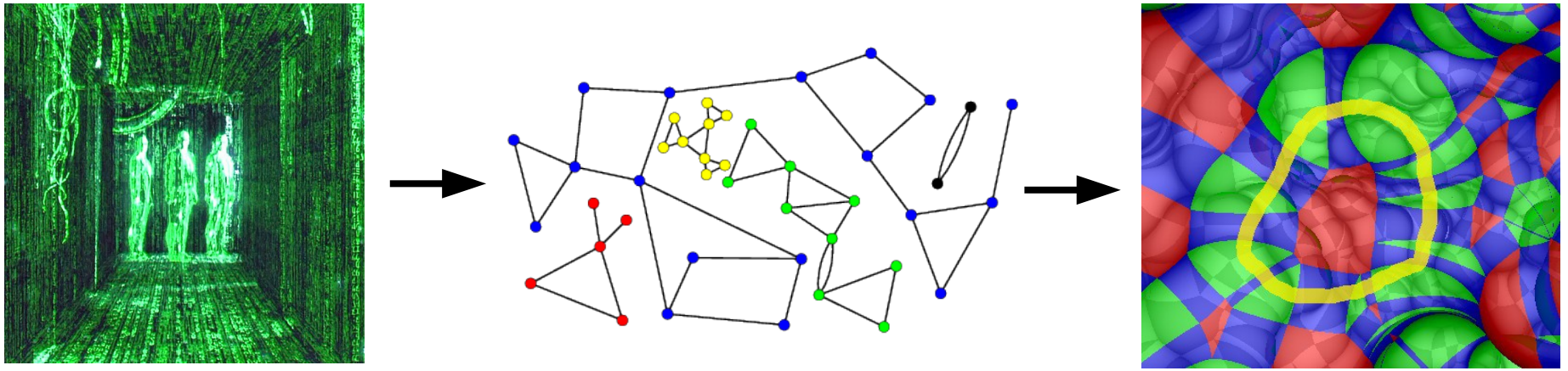
  2) Triangles connected with tori

  - Spherical polygons enclosed with tori
  - Benefit – every vertex has three edges



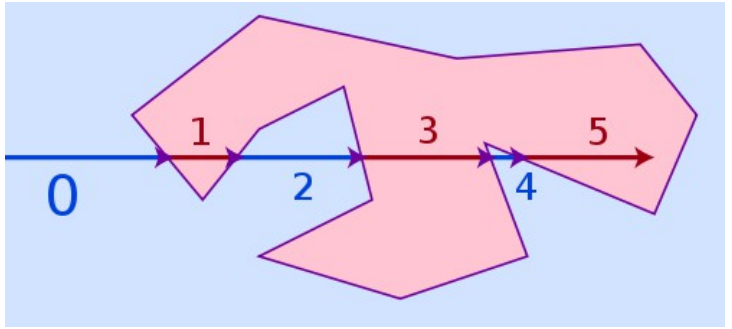
Surface Graph – Implementation

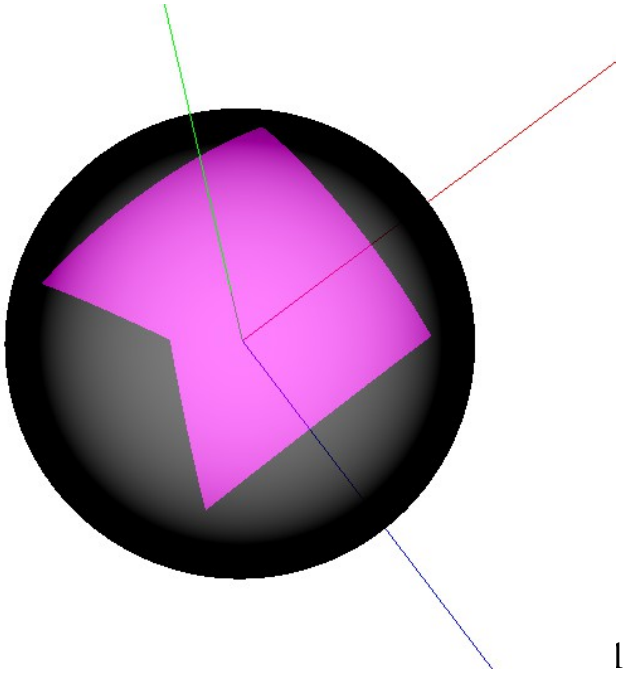
- CB modifications – output SG edges
- CC analysis – on GPU:
  1) Build adjacency matrix
  2) Label components – parallel BFS
  3) Find polygon circles – CC again



Rendering Spherical Polygons

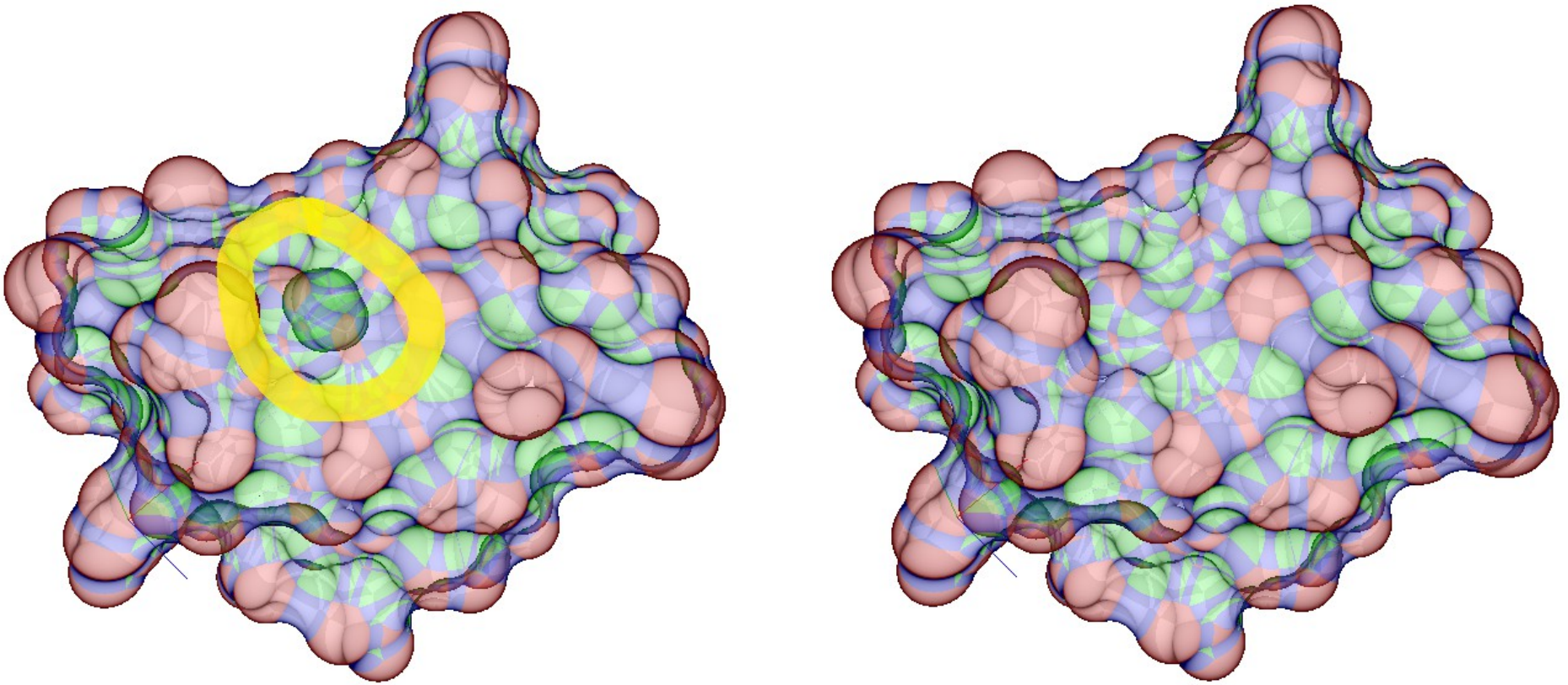
- Spherical geometry
  - Surface of sphere
  - Every two lines (great circles) intersect
- SES patches = polygons
  - Lines on sphere (small circles)
  - Odd-even rule + point outside





Results I

- Visualization of 1CRN (PDB)
  - 327 atoms, transparent SES – probe 1,4 Å



Results II

- Performance comparison (FPS@1024x1024)

	Solvent excluded surface (SES)				Solvent accesible surface (SAS)			
PDB	1YV8		1VIS		1YV8		1VIS	
Atoms	641		2482		641		2482	
Coverage	18,0 %		48,0 %		23,0 %		55,4 %	
Method	our	Kauker	our	Kauker	our	Kauker	our	Kauker
GTX 580	**18,3**	31,0	**7,3**	11,2	**17,8**	14,7	**7,4**	4,8
GTX 680	**32,3**	22,1	**13,9**	7,7	**33,2**	10,3	**14,9**	3,3
R9 270X	19,8	-	9,4	-	20,5	-	10,1	-
GTX 980	48,3	-	21,8	-	49,8	-	22,5	-

Conclusion

- Contribution
  - Novel and faster transparent dynamic SES/SAS visualization method
  - OpenGL 4.3 implementation – nVIDIA, ATI
- (Near) Future work
  - Bug fixing – 2 known bugs
  - Publication

Thank you for your attention!