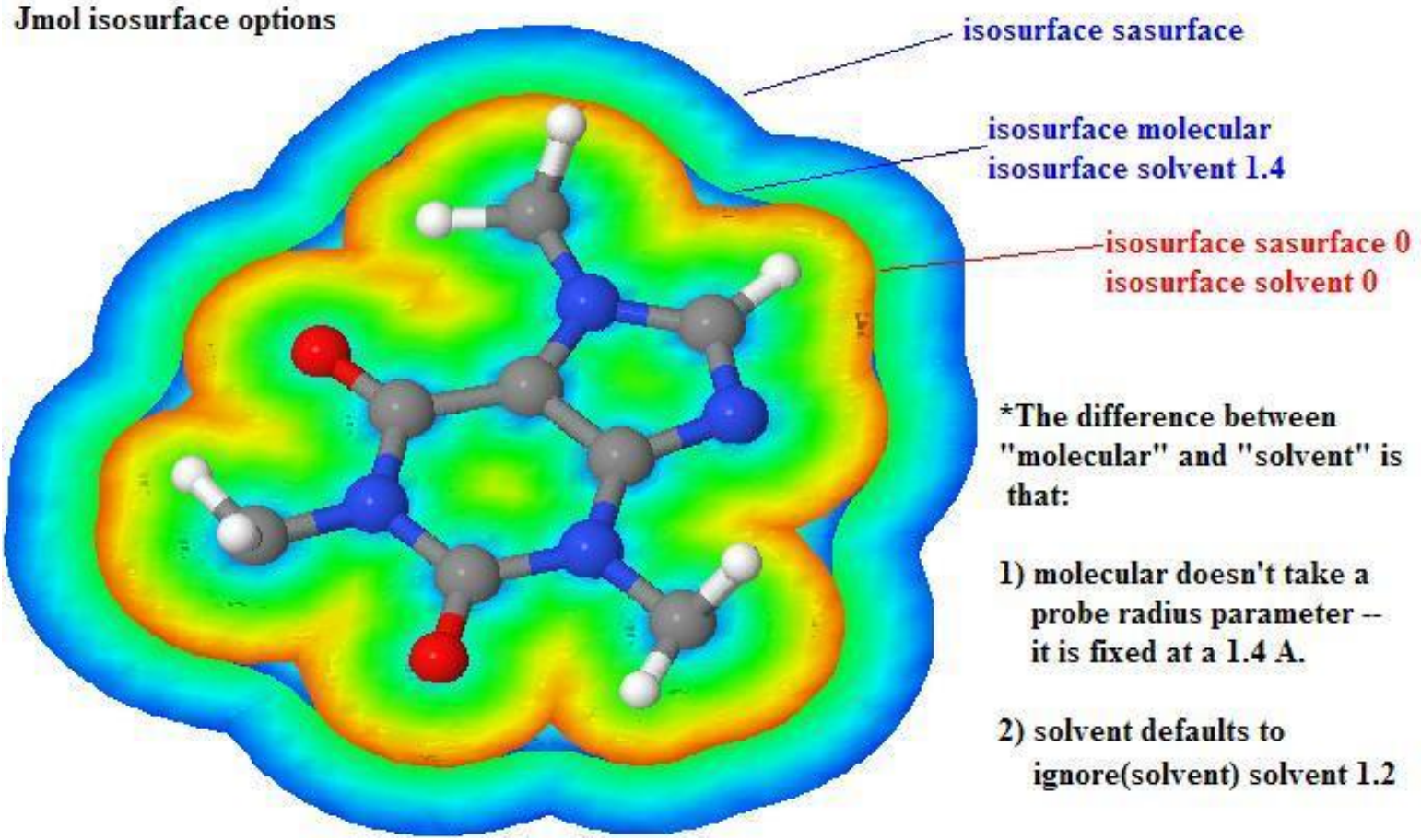
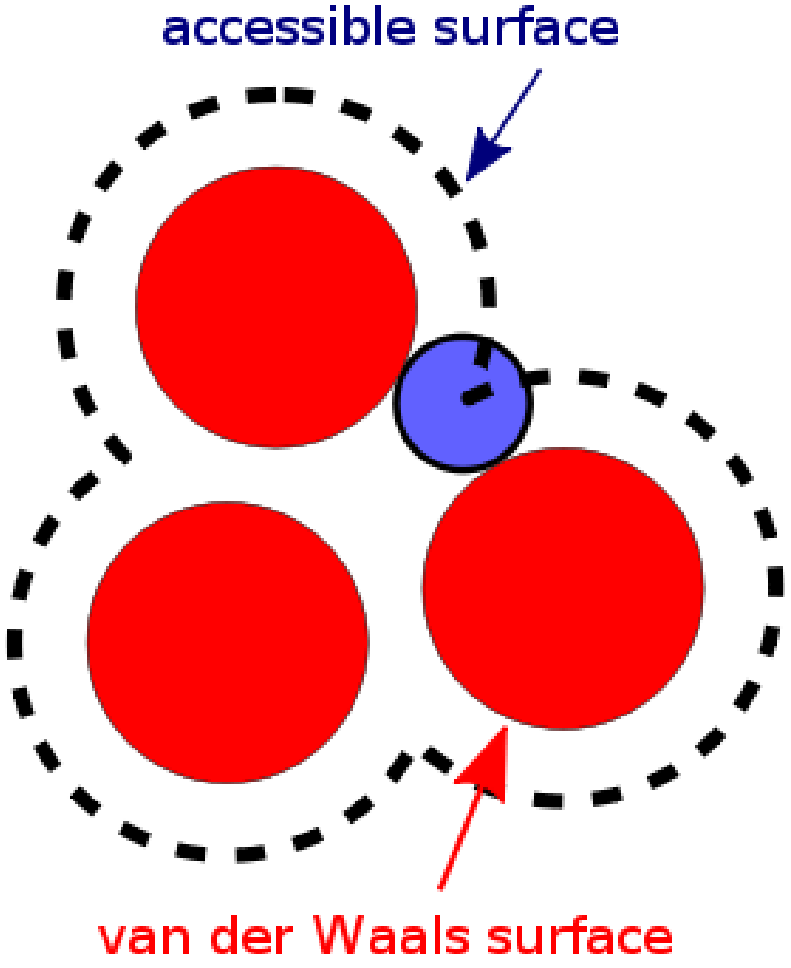
Lecture 16

Molecular Surface

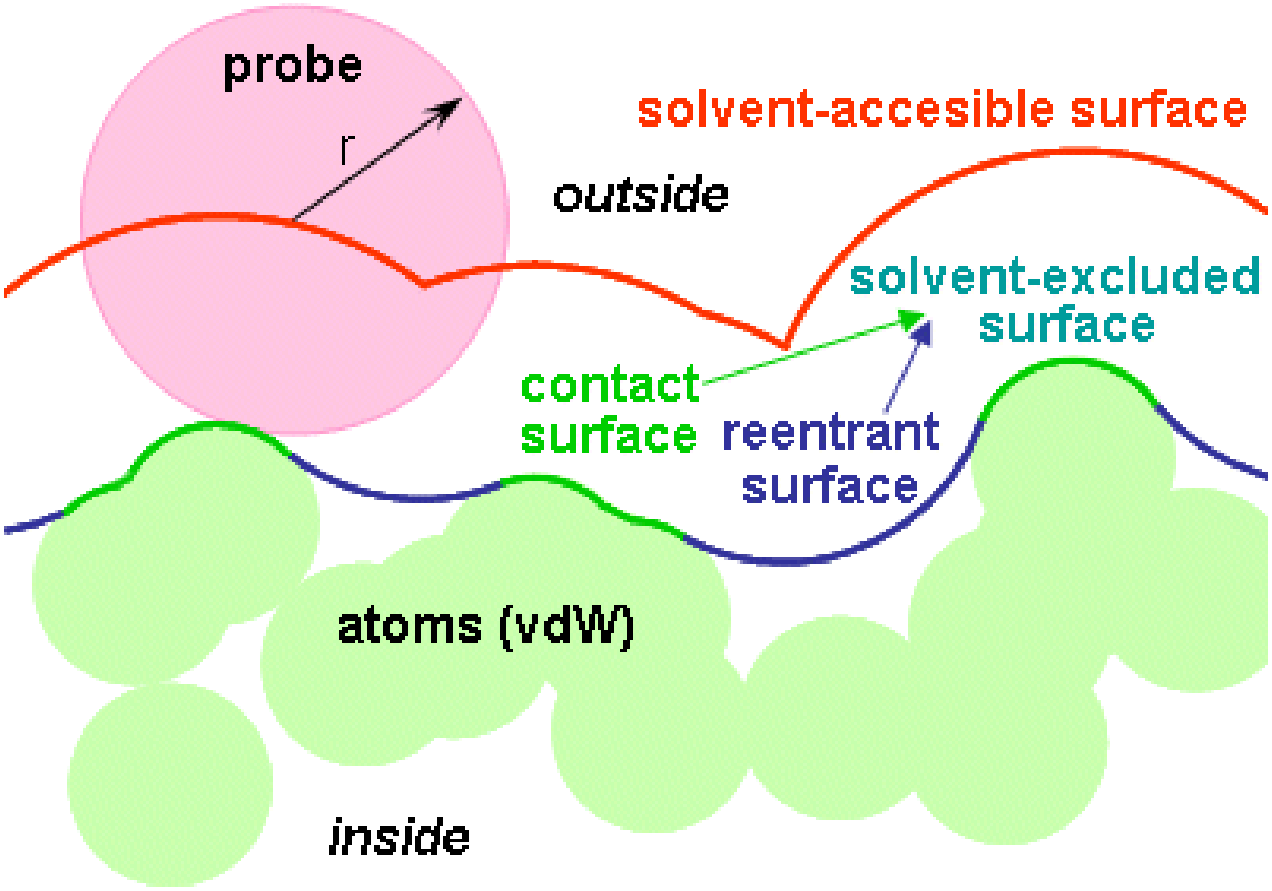
Molecular Surface



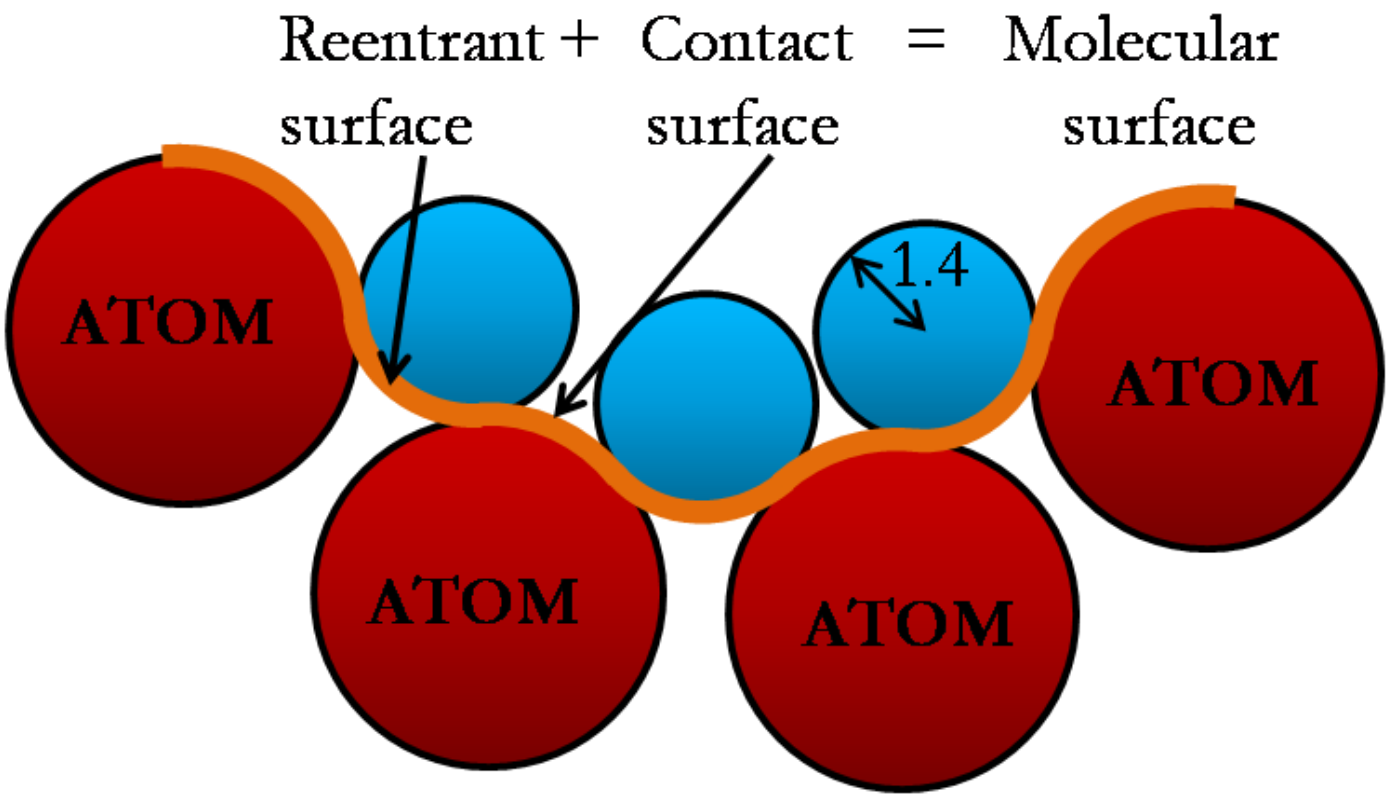
Molecular Surface



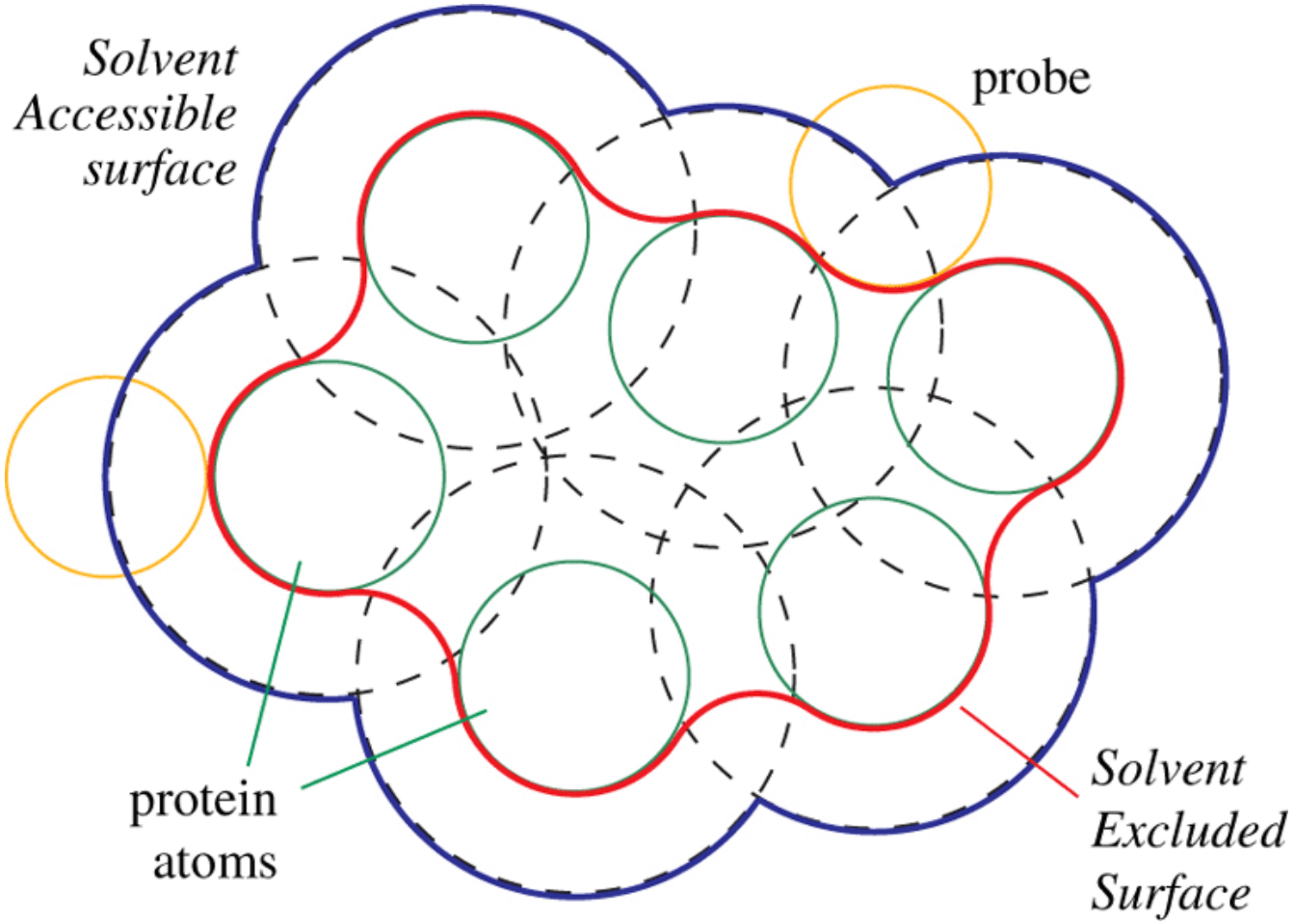
Molecular Surface



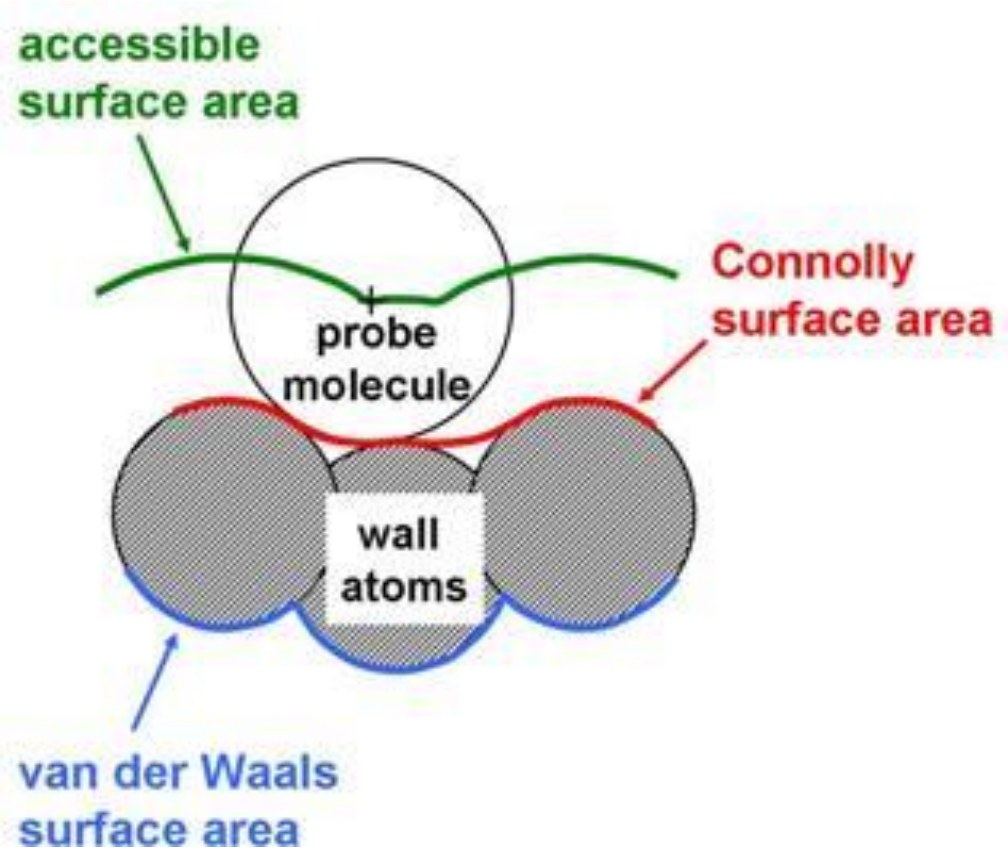
Molecular Surface



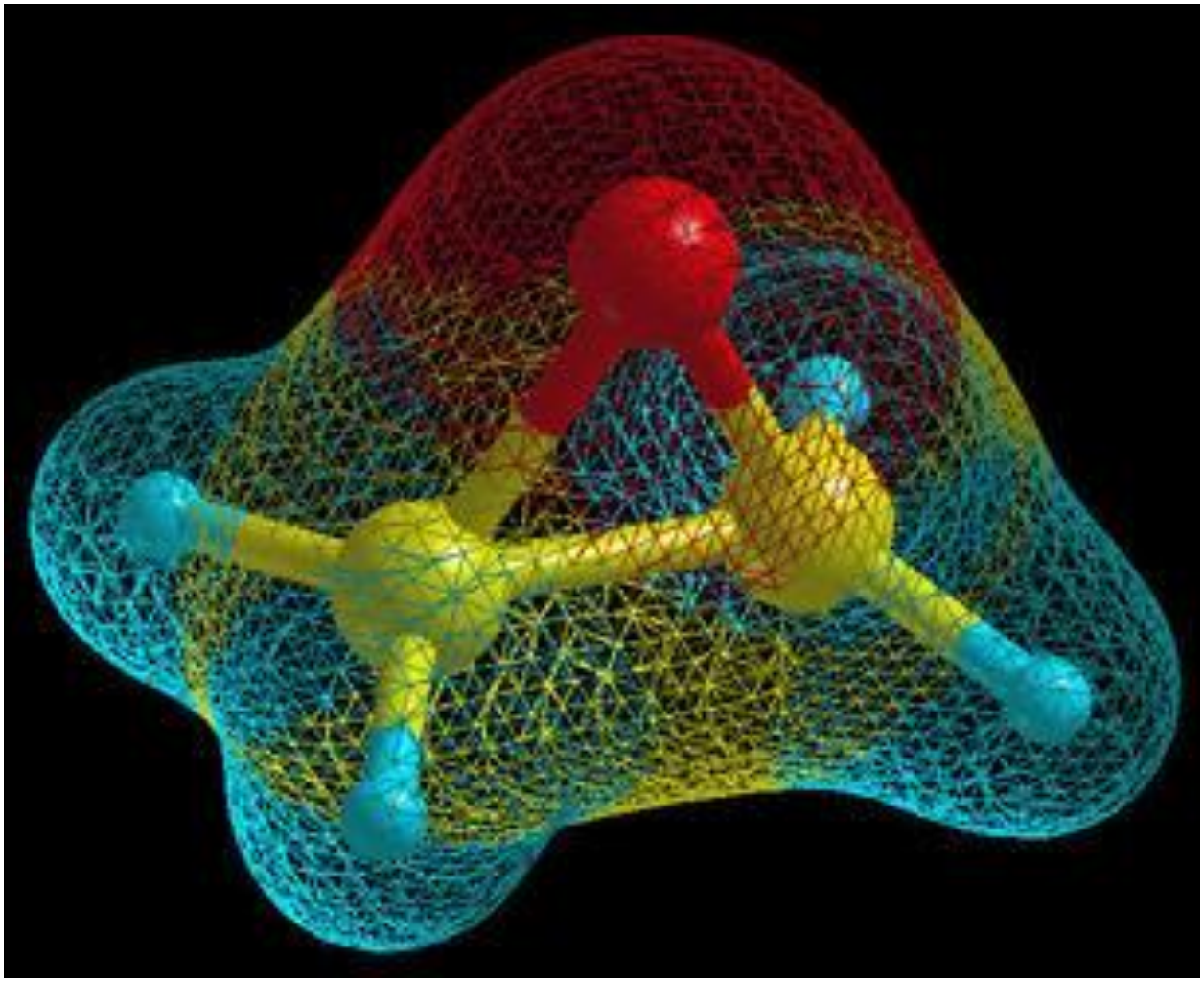
Molecular Surface



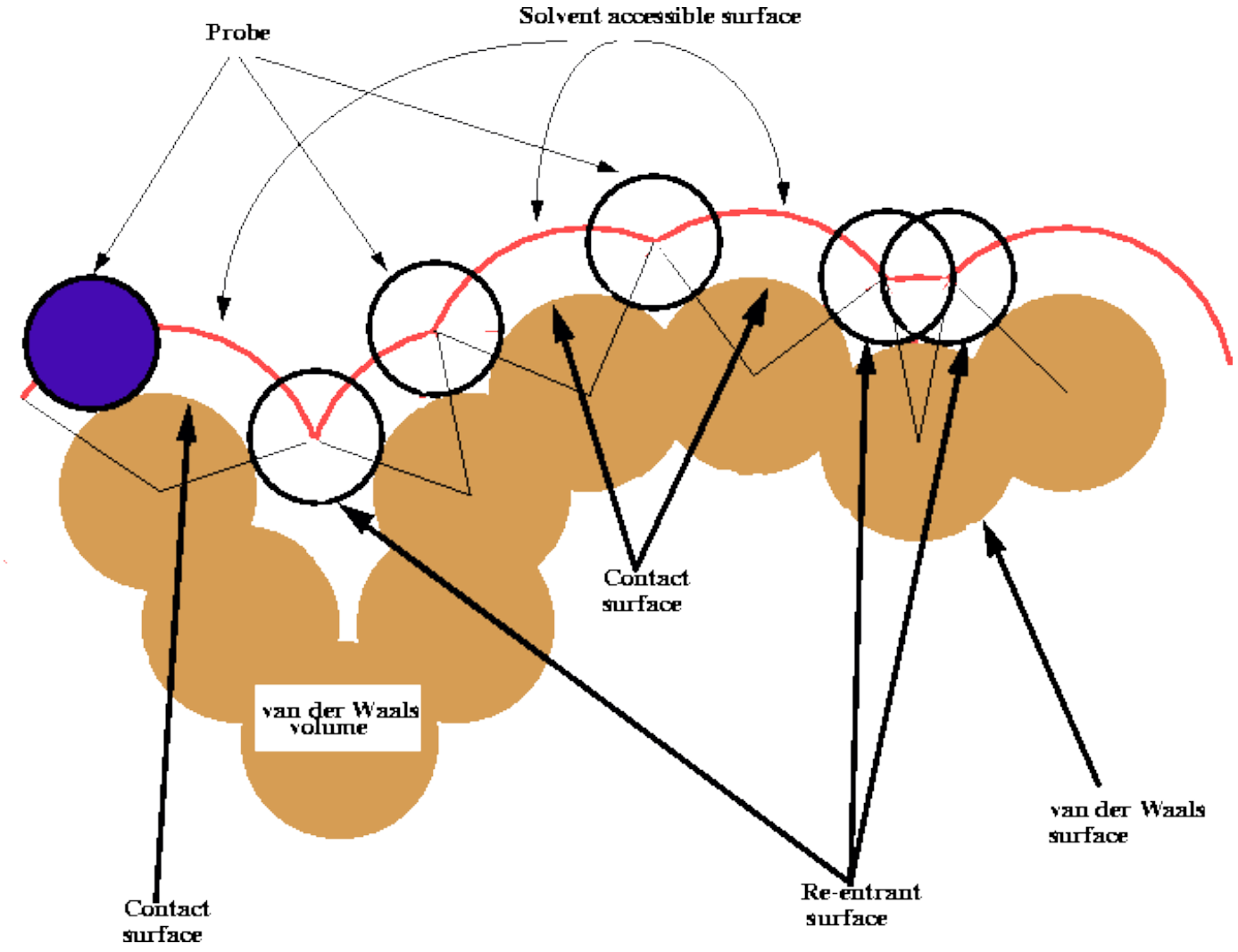
Molecular Surface



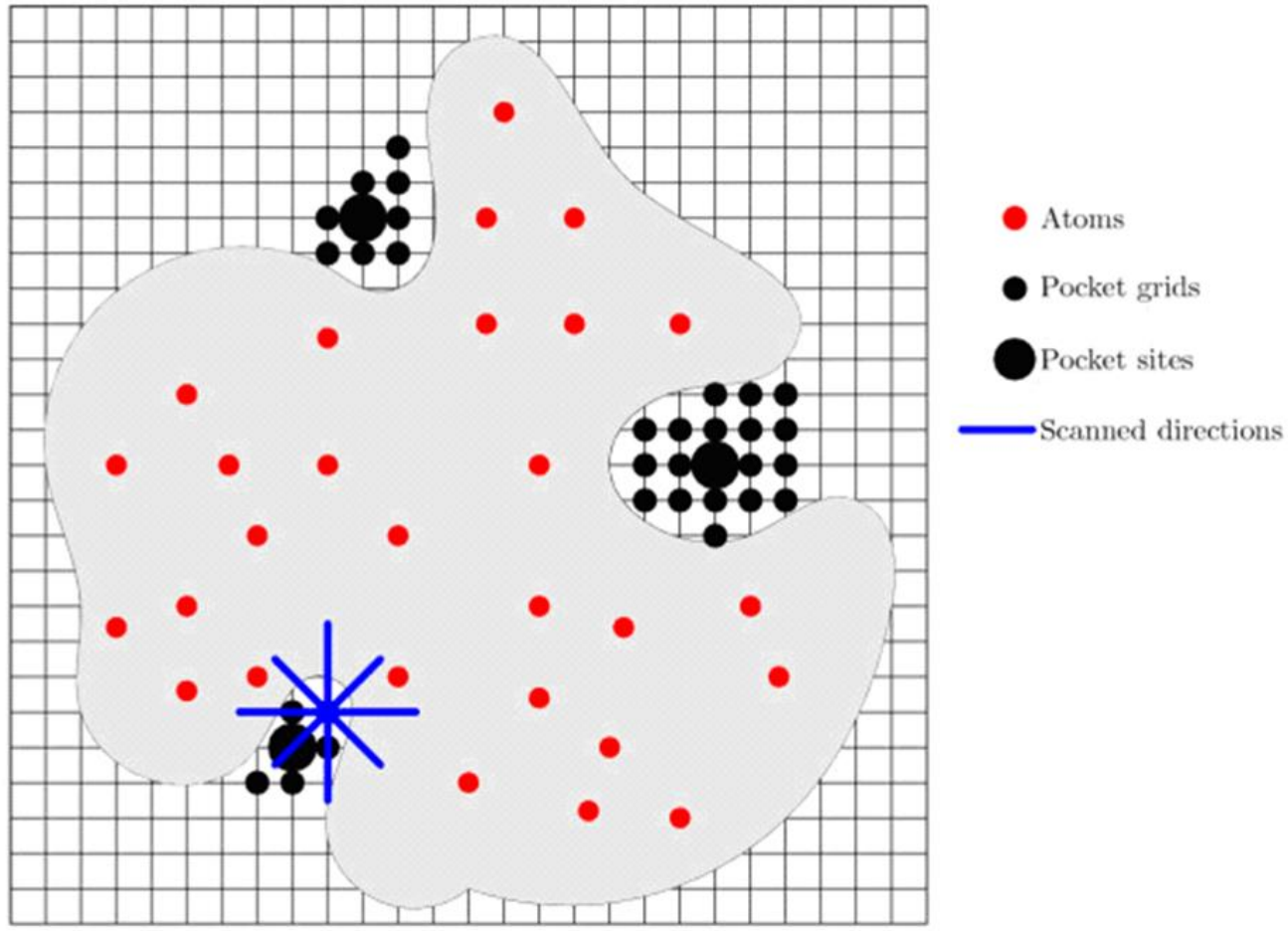
Molecular Surface



Molecular Surface



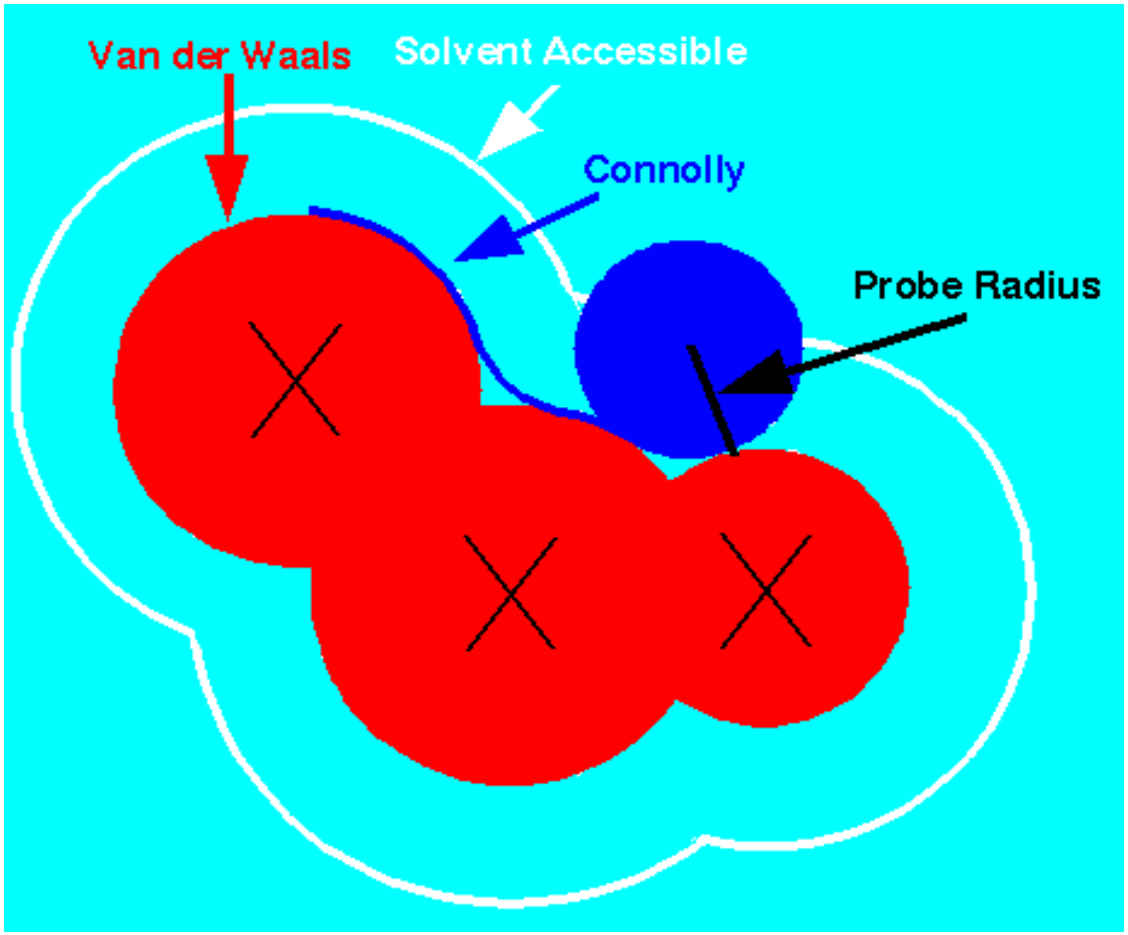
Molecular Surface



Mathematical Models of Surface Representation

- Connolly surface
- NACCESS
- Surface Normal and Critical Points
- Grid Representation
- Advantage
    - Geometric Hashing based rigid-body programs

Solvent Accessible Surface – SAS
Connolly Surface



Connolly's MS algorithm

- A 'water' probe ball (1.4-1.8 A diameter) is rolled over the van der Waals surface.

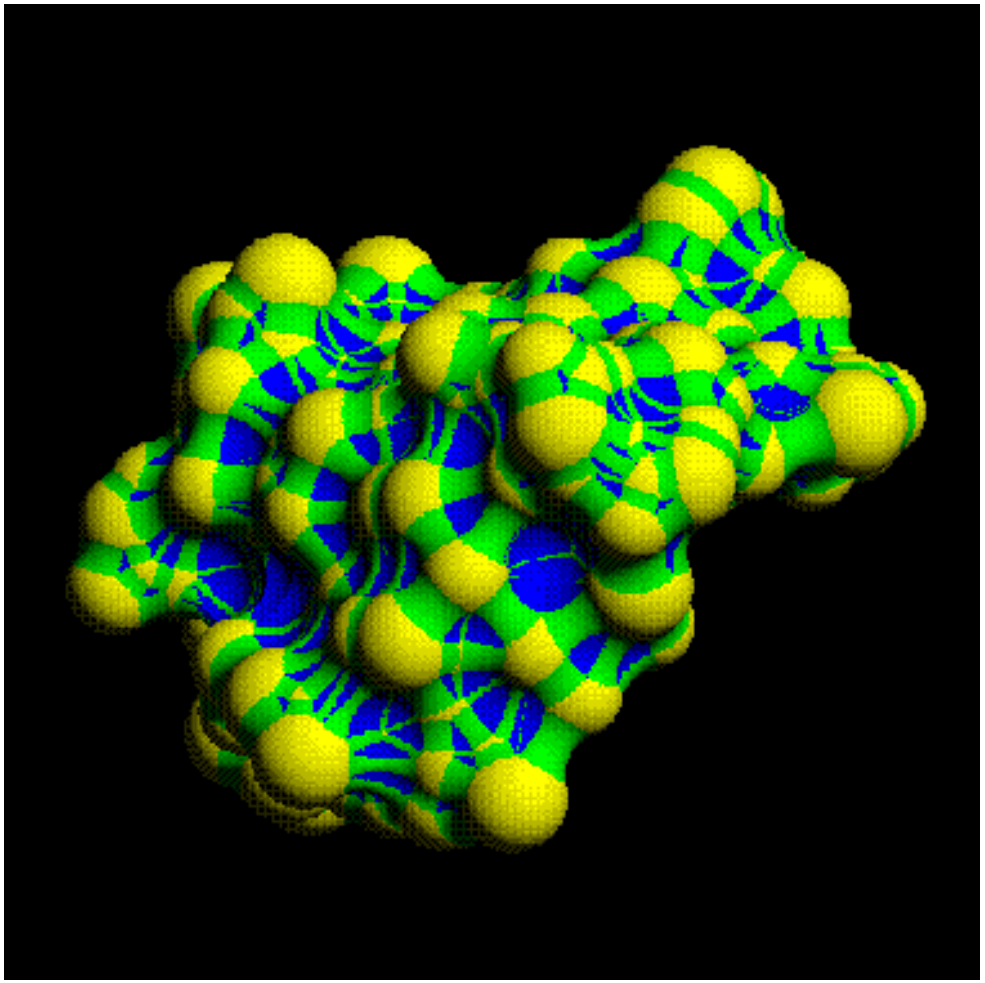
- Smoothens the surface and bridges narrow 'inaccessible' crevices.

Connolly's MS algorithm - cont.

- Convex, concave and saddle patches according to the no. of contact points between the surface atoms and the probe ball.

⌗ Outputs points+normals according to the required sampling density (e.g. 10 pts/A^2).

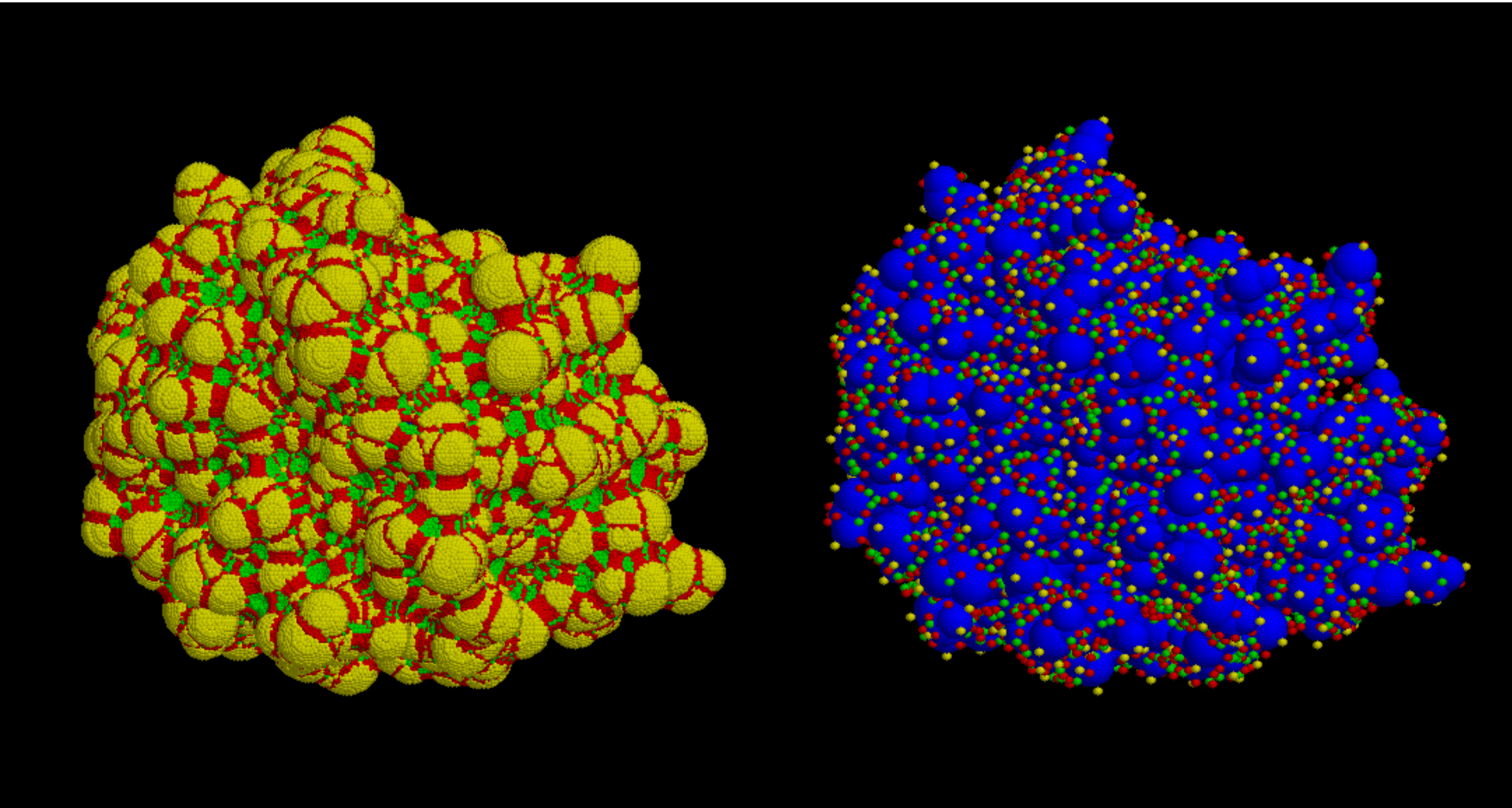
Example - the surface of crambin



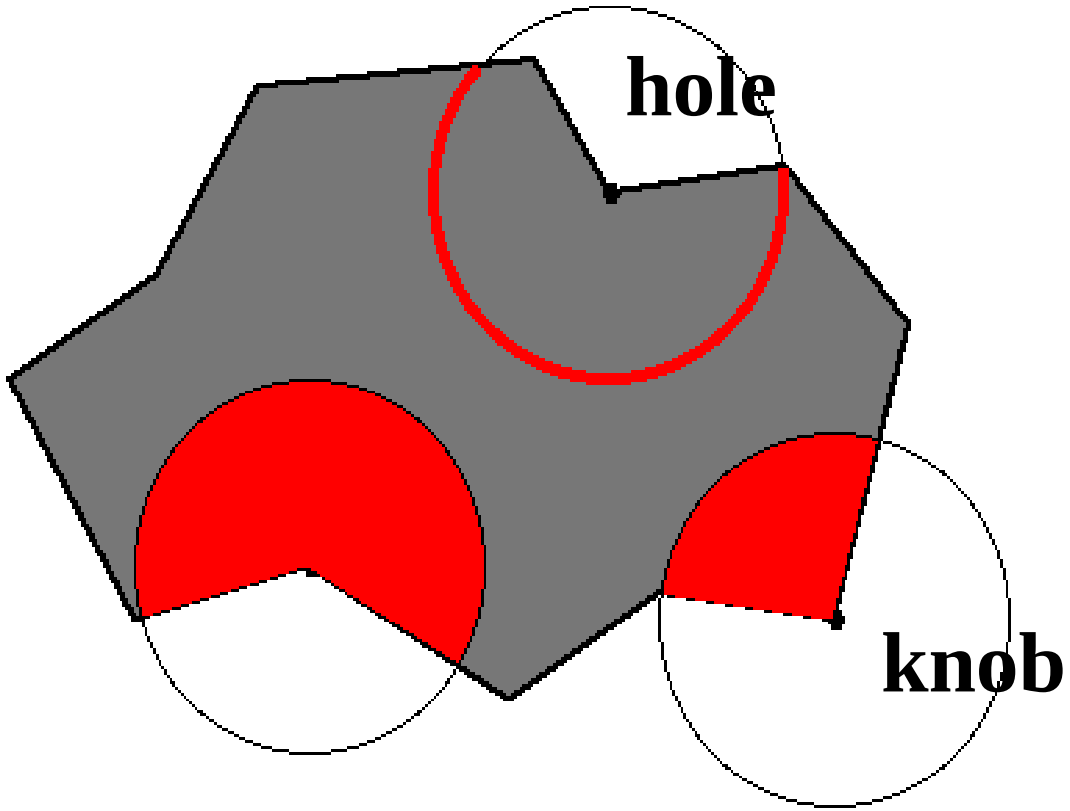
Critical points based on Connolly rep. (Lin, Wolfson, Nussinov)

- Define a single point+normal for each patch.
- Convex-caps, concave-pits, saddle - belt.

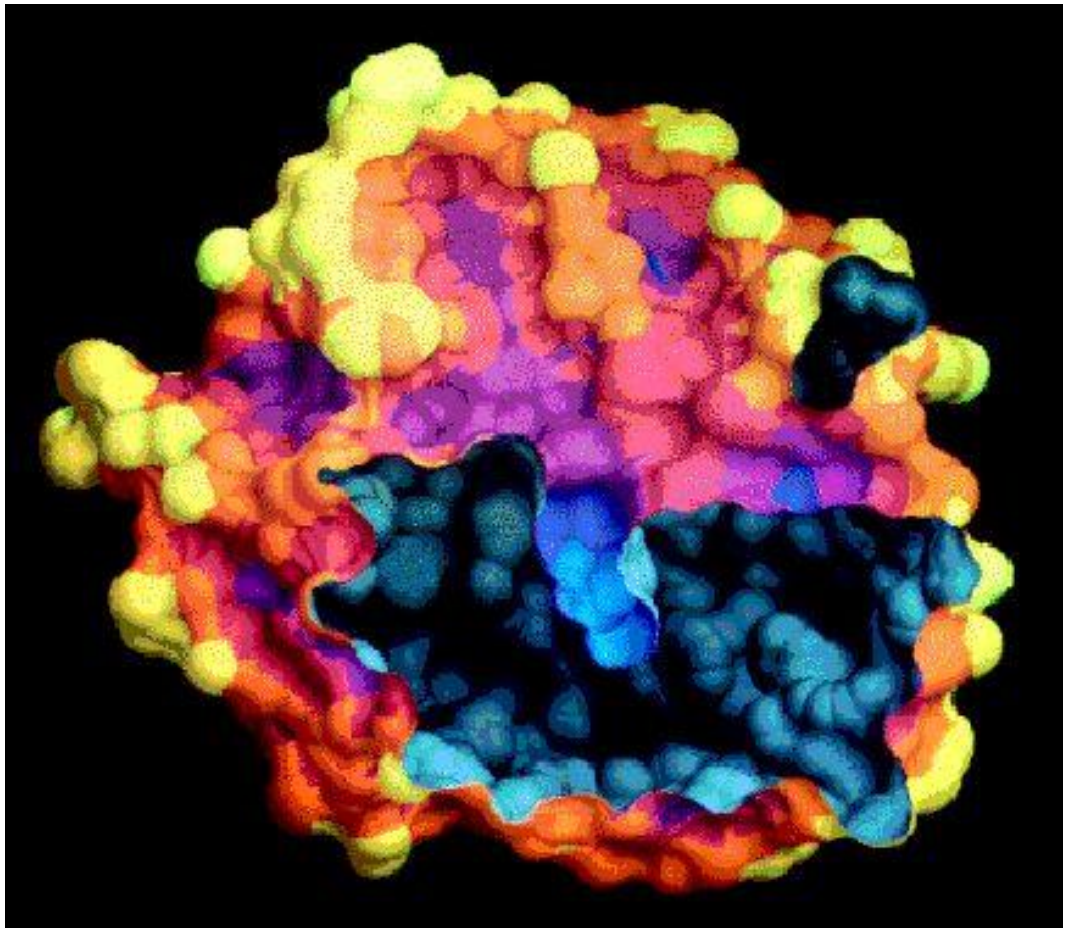
Connolly => Shou Lin



Solid Angle local extrema



Chymotrypsin surface colored by solid angle (yellow-convex, blue-concave)



Definition of Protein Surface

- Roll the probe over the protein molecule using NACCESS program to compute the accessible surface area (ASA) (also called as SASA – surface accessible surface area)

- If an atom's accessible surface area (ASA) is more that 0.1 $Å^2$ then that is define as surface atom.

Definition of Protein Interface Area

- The surface area where two protein molecules interacts during complex formation is called as the interface region.

- If an atom loses its ASA by more than 0.1 $Å^2$ then we call that as an interface atom. The total loss of ASA by all the interface atoms are the interface area.

- Sometimes, we take the average for interface area to call it as interface area per protein molecule.

- How to compute identify interface atoms? How to compute interface area?
  - Run the NACCESS on individual protein molecules
  - Run the NACCESS on the protein complex
  - Identify the atoms that loses its ASA by more than 0.1 $Å^2$

Definition of Protein Interface Area