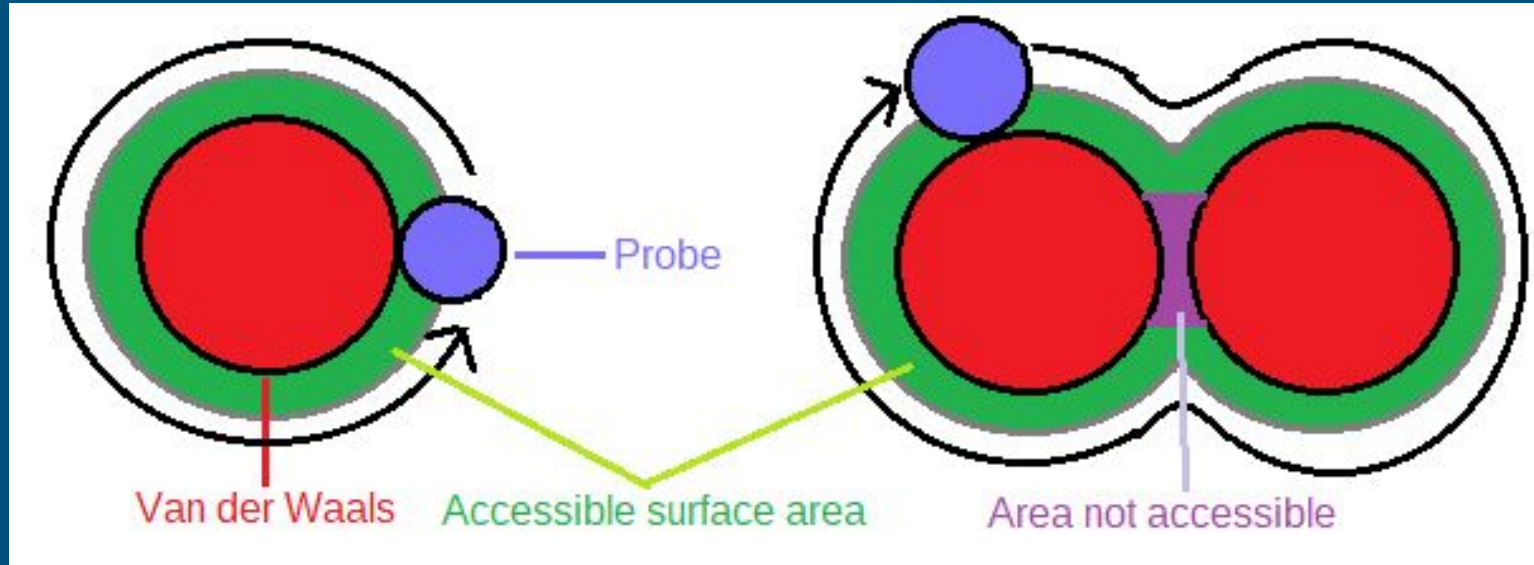


Calculating the accessible surface area of a protein

By Bel Alexis
2022-2023

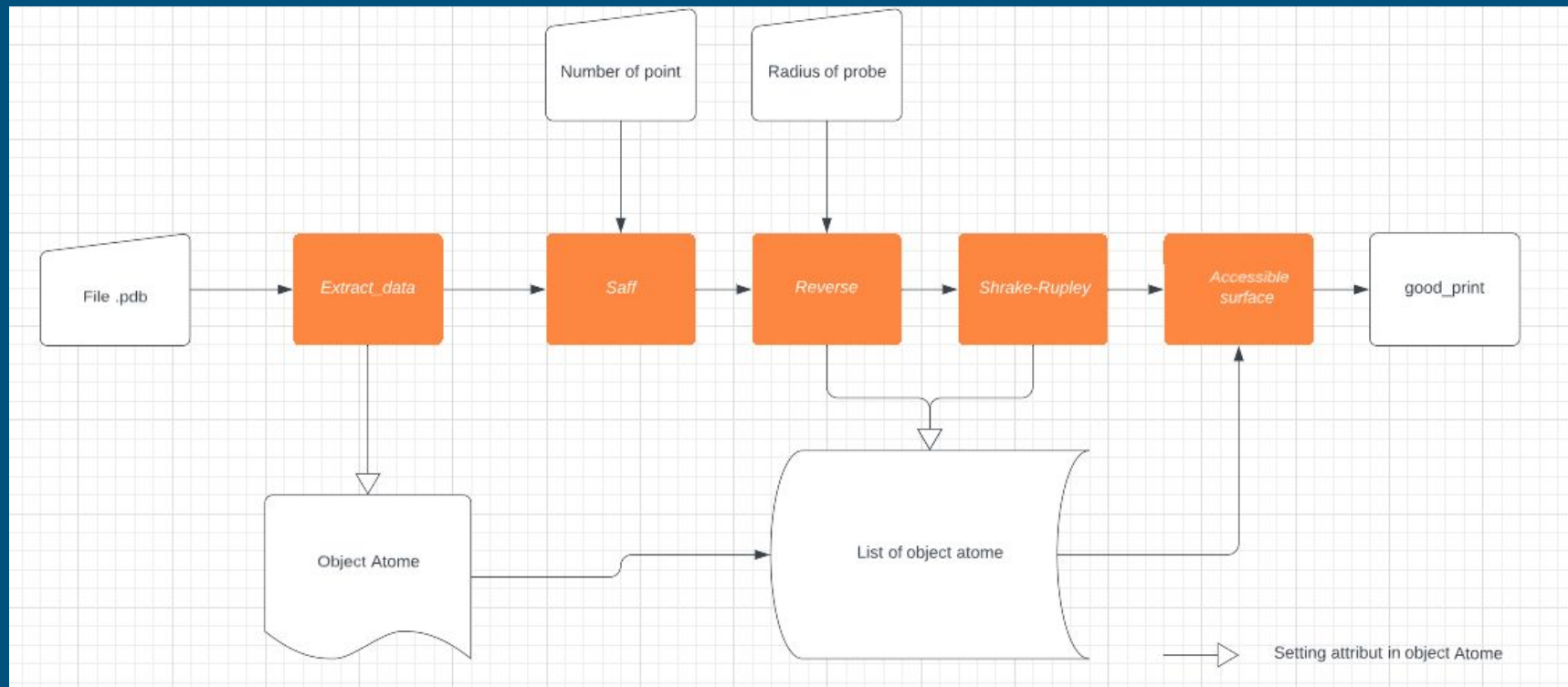
Shrake, A; Rupley, JA. (1973). "Environment and exposure to solvent of protein atoms. Lysozyme and insulin". J Mol Biol 79 (2): 351–71. doi: 10.1016/0022-2836(73)90011-9.

What is ASA?

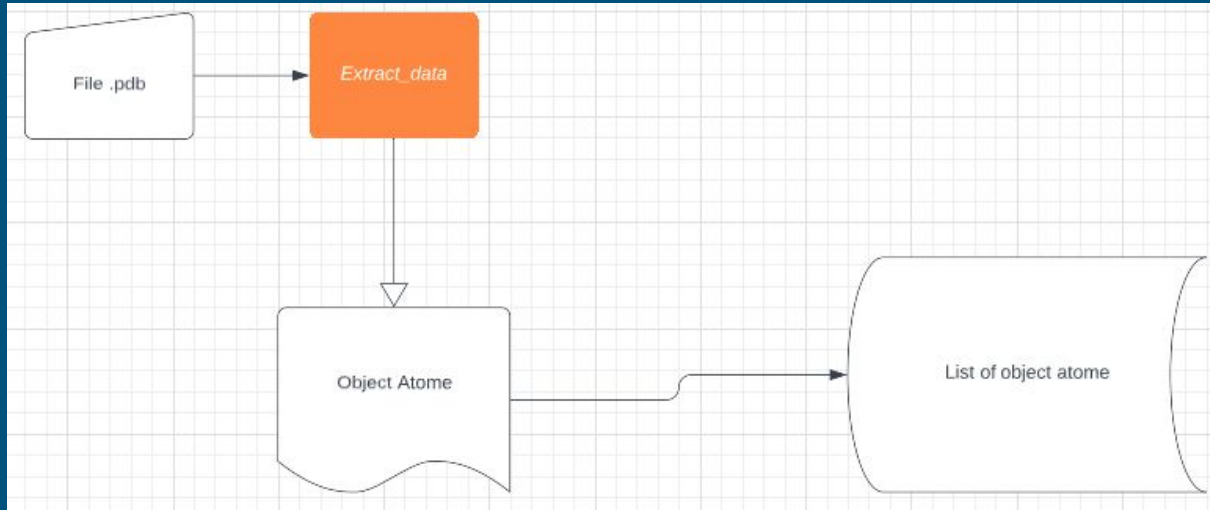


Picture of the algorithm of Shrake Rupley

Pipeline

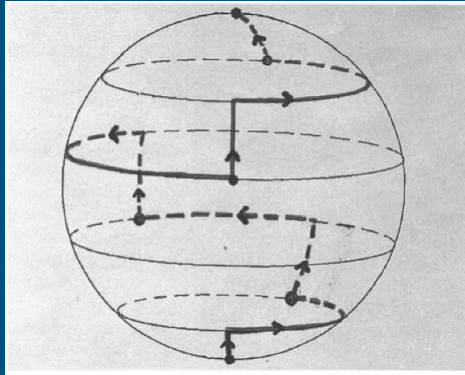
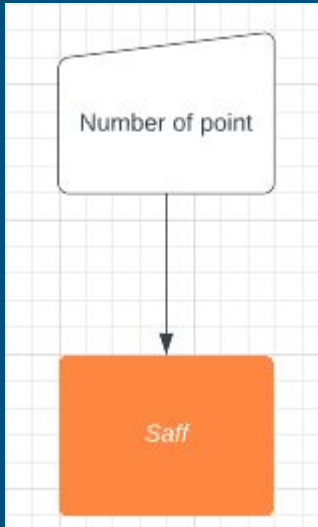


Pipeline extraction

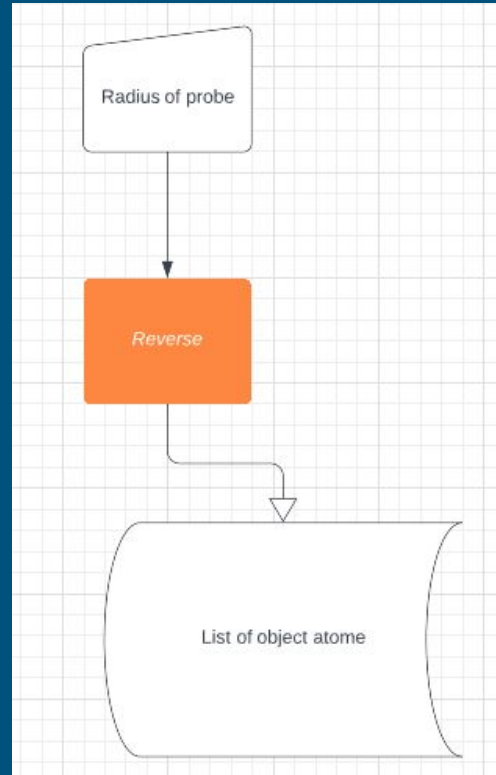


- Extract data from a .pdb
- For each atom a object atom is creates
- A list contain all the object atom

Pipeline: Saff et reverse

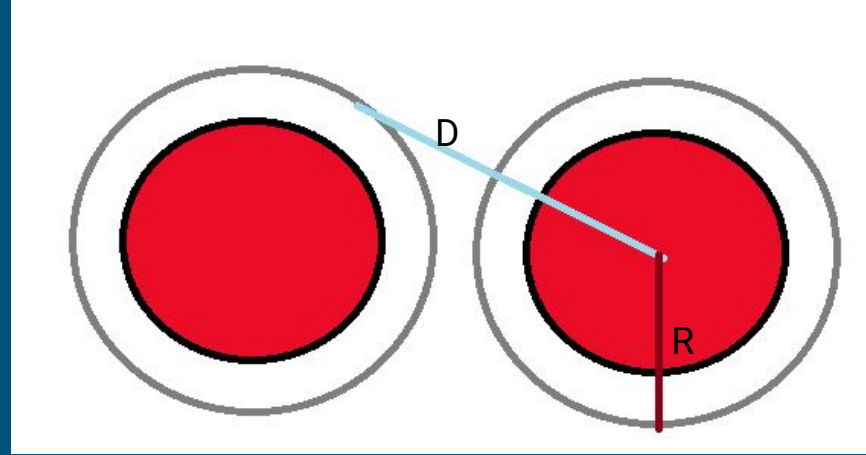
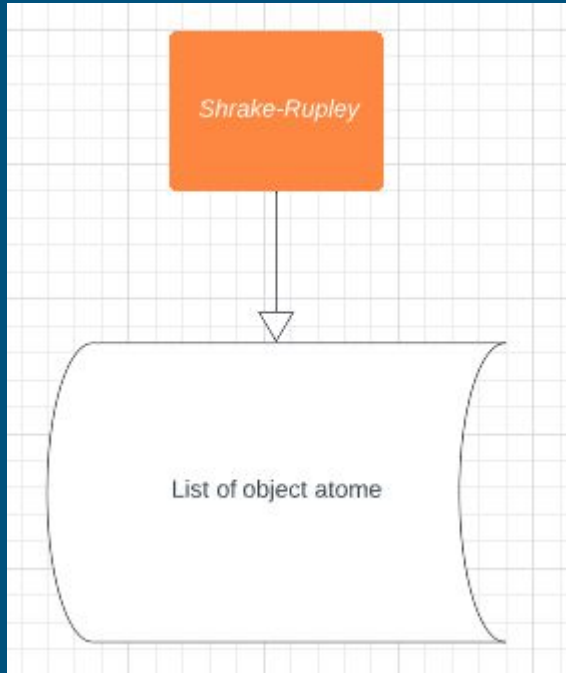


Saff, E.B., Kuijlaars, A.B.J. Distributing many points on a sphere. *The Mathematical Intelligencer* 19, 5–11 (1997).
<https://doi.org/10.1007/BF03024331>



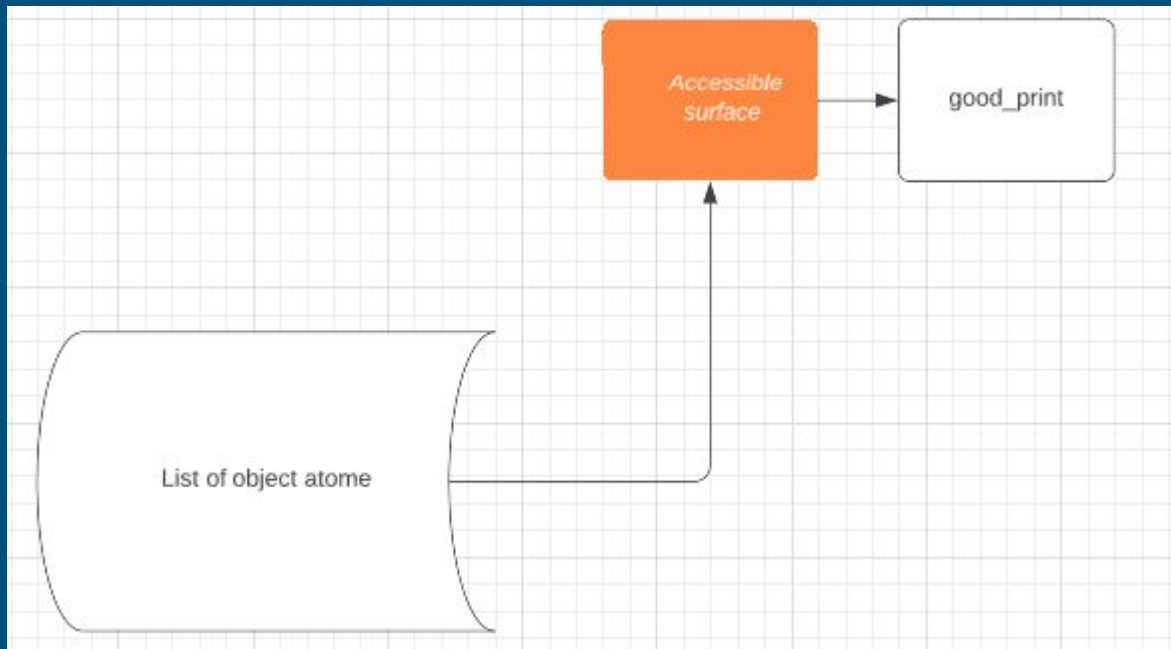
- Spherical coordinate to 3d coordinates
- 3d coordinates in object atom

Pipeline: Shrake Rupley



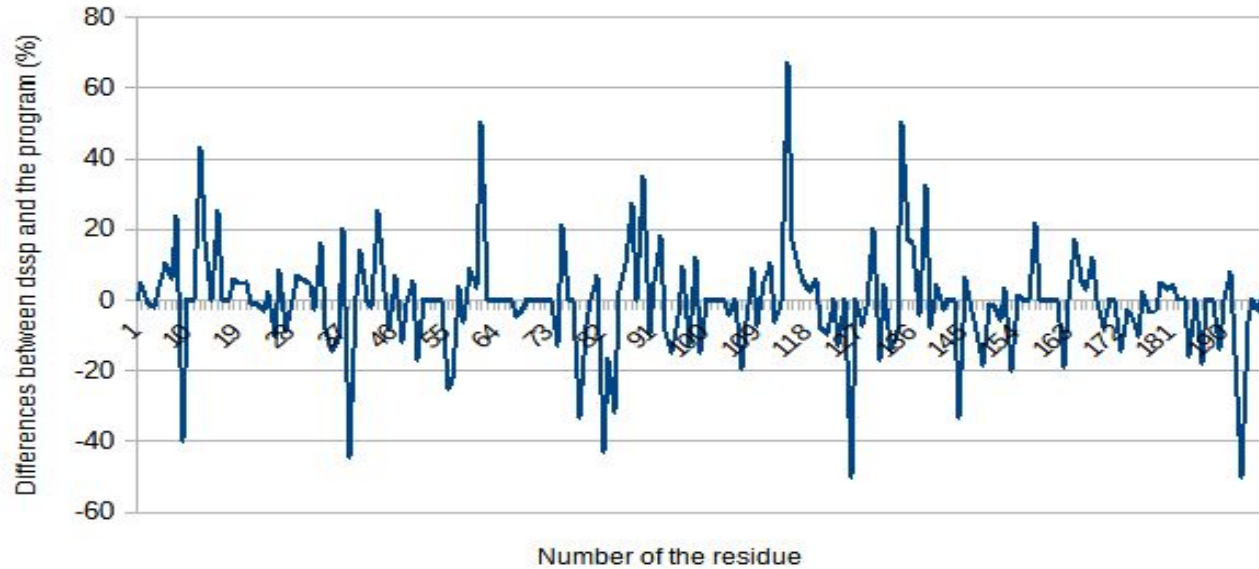
Compare D and R to determine if a point is buried or not

Pipeline: Accessible surface



- Add the ASA of atom by residue
- Add the ASA of All residue
- Add the maxASA of all residue
- Ratio of Sum of ASA / Sum MaxASA

Result:



Mean of the differences : -0.3%
Script = 9730 A²
DSSP = 9623 A²

28 % of the protein is accessible

Difference between the results obtain by dssp and by the program

Discussion:

- Working program
- Testing on larger protein
- Multiprocessing



Thank you for your attention