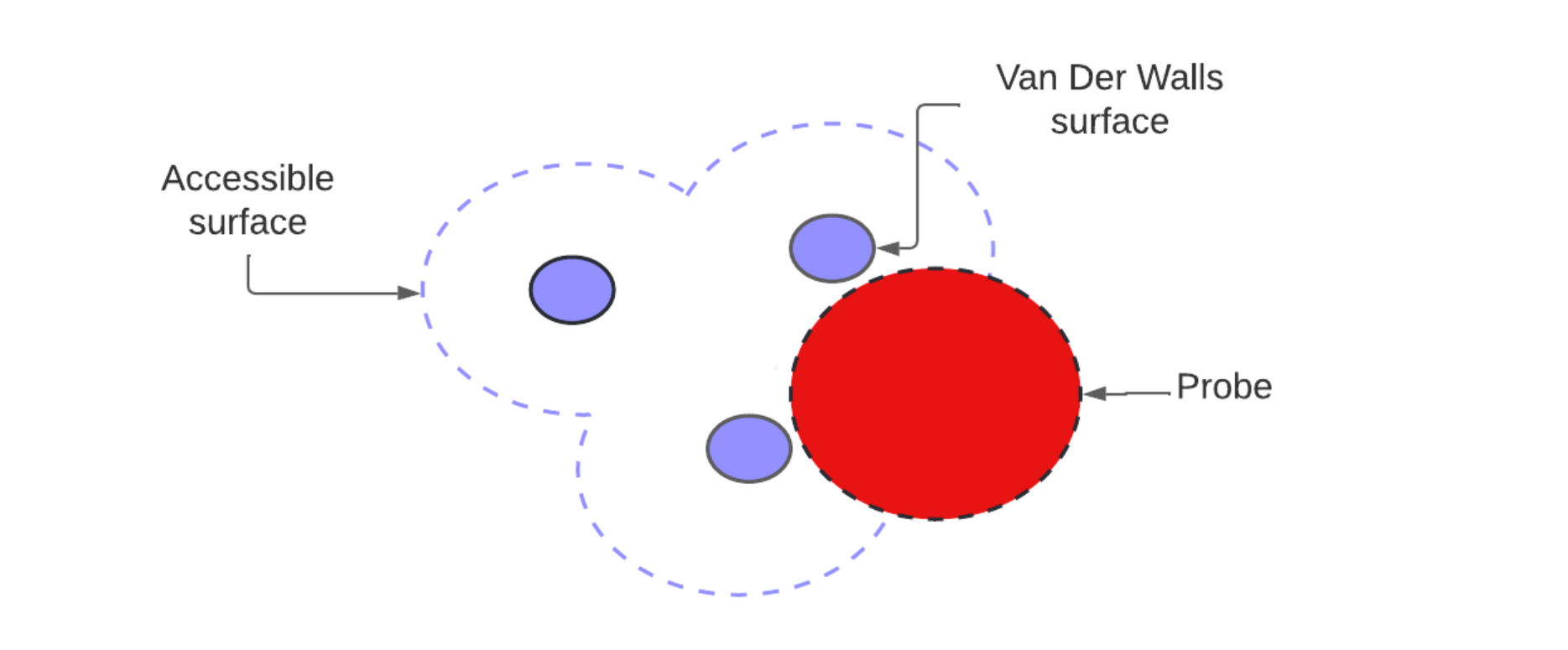
Université Paris Cité

Calculation of the solvent accessible surface of a protein

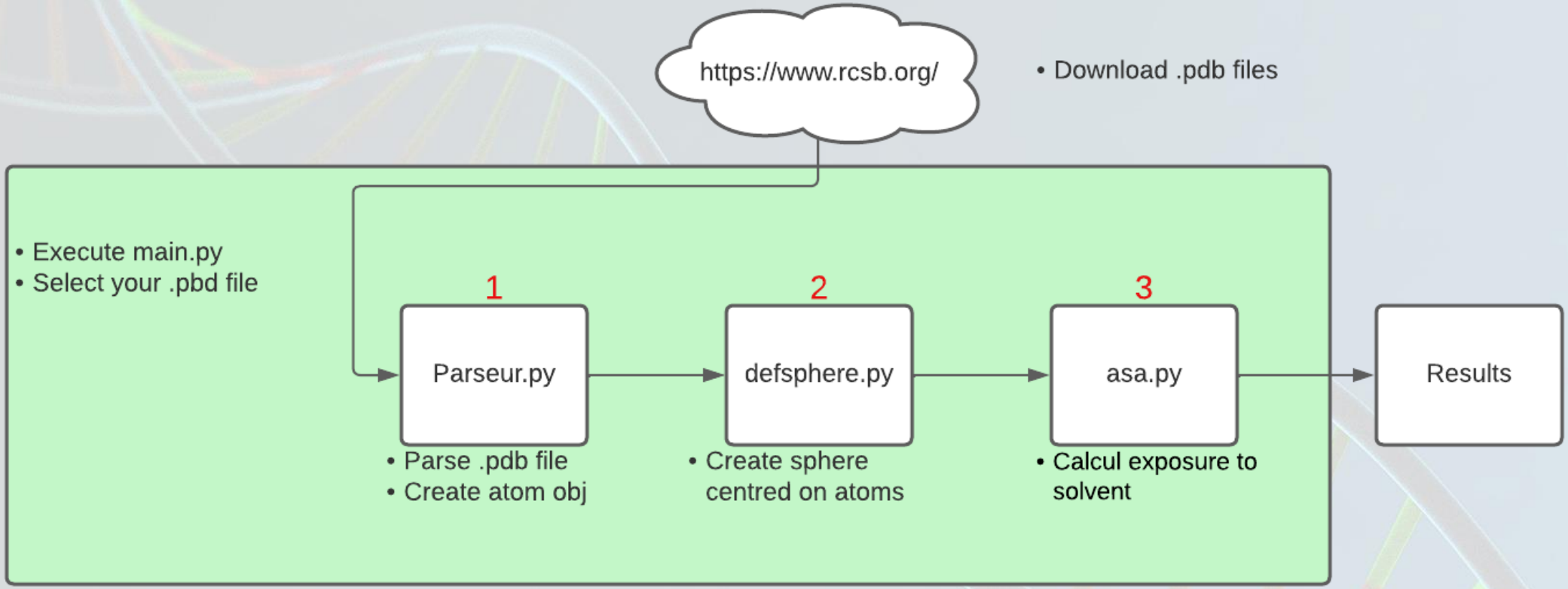
Anas BELAKTIB

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?



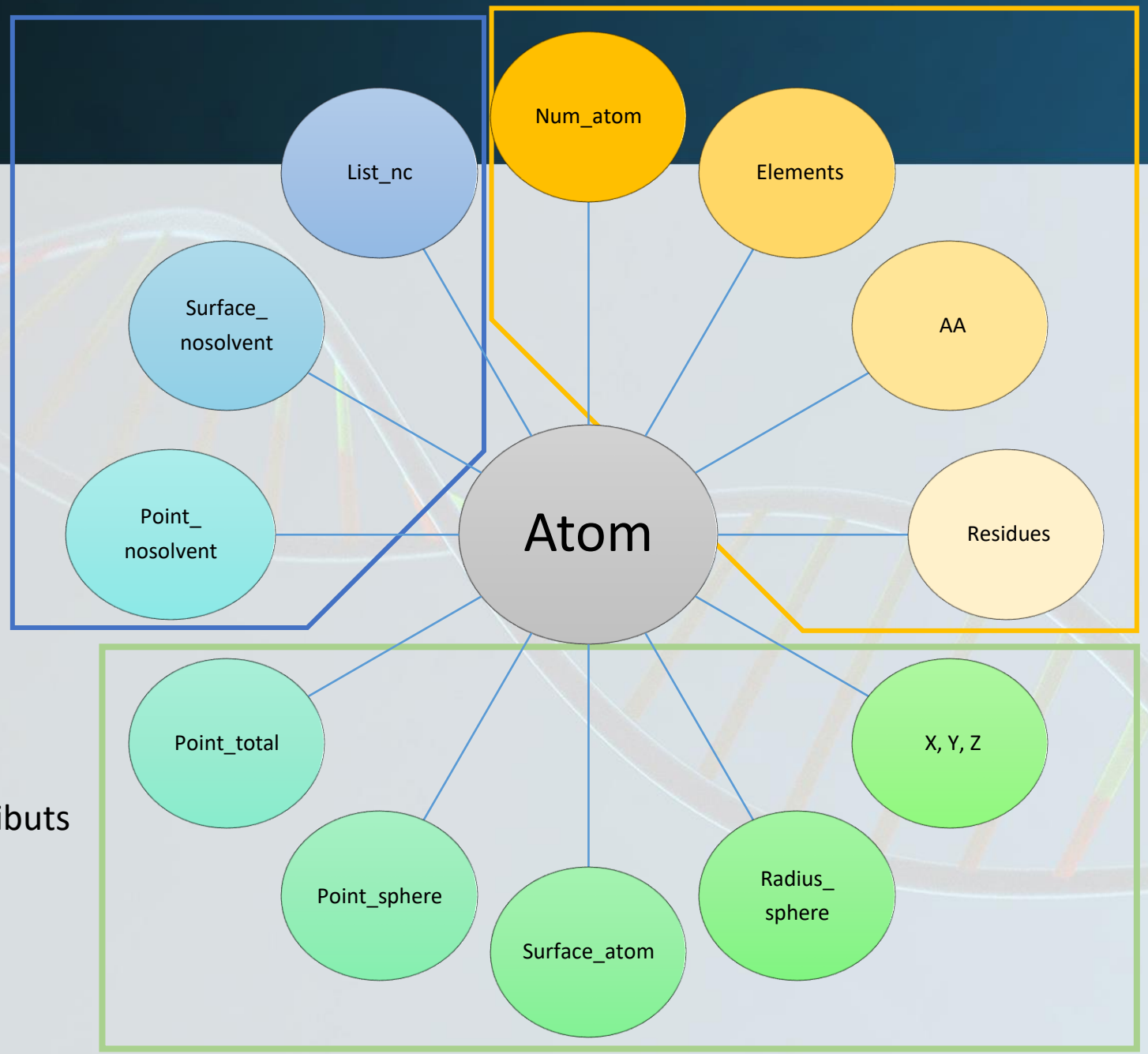
Pipeline



DEPEDENCIES :

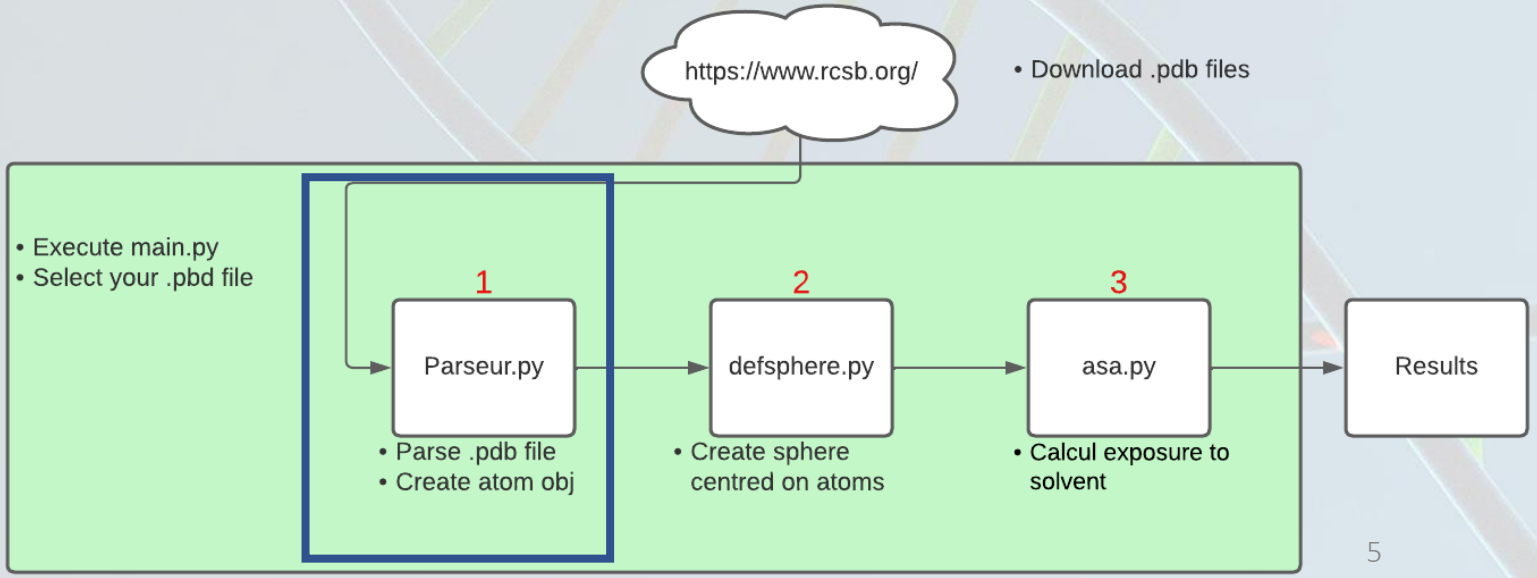
- Python
- Biopython
- .pdb files

OOP


ASA attributs
Atom ID attributs
Space attributs
List_nc
Num_atom
Elements
Surface_ nosolvent
AA
Point_ nosolvent
Atom
Residues
Point_total
X, Y, Z
Point_sphere
Surface_atom
Radius_ sphere

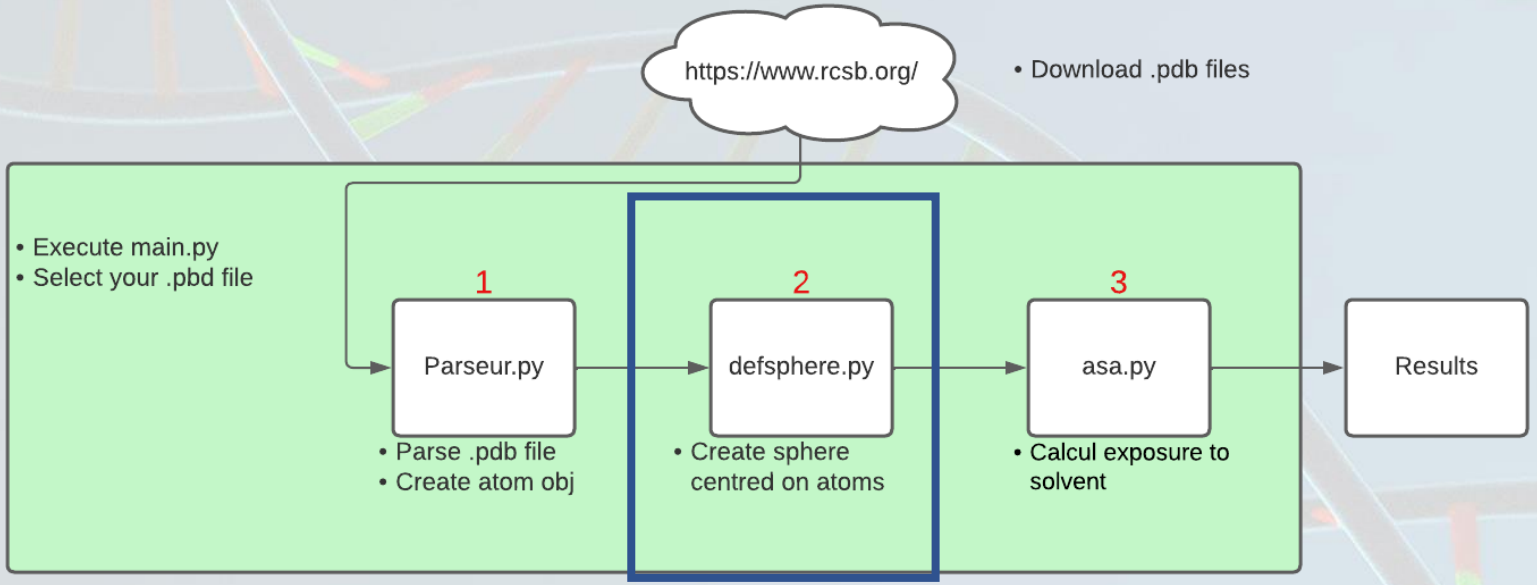
Parse .pdb files

- *RCBS Protein Data Bank [2]*
- *Biopython*
- *Only lines starting with ATOM*
- *Only the first model*



Create Sphere

- *Fibonacci algorithm*
- *92 points **[3]***
- *Radius for each atom + VdW radius*
- *Adjusted center*



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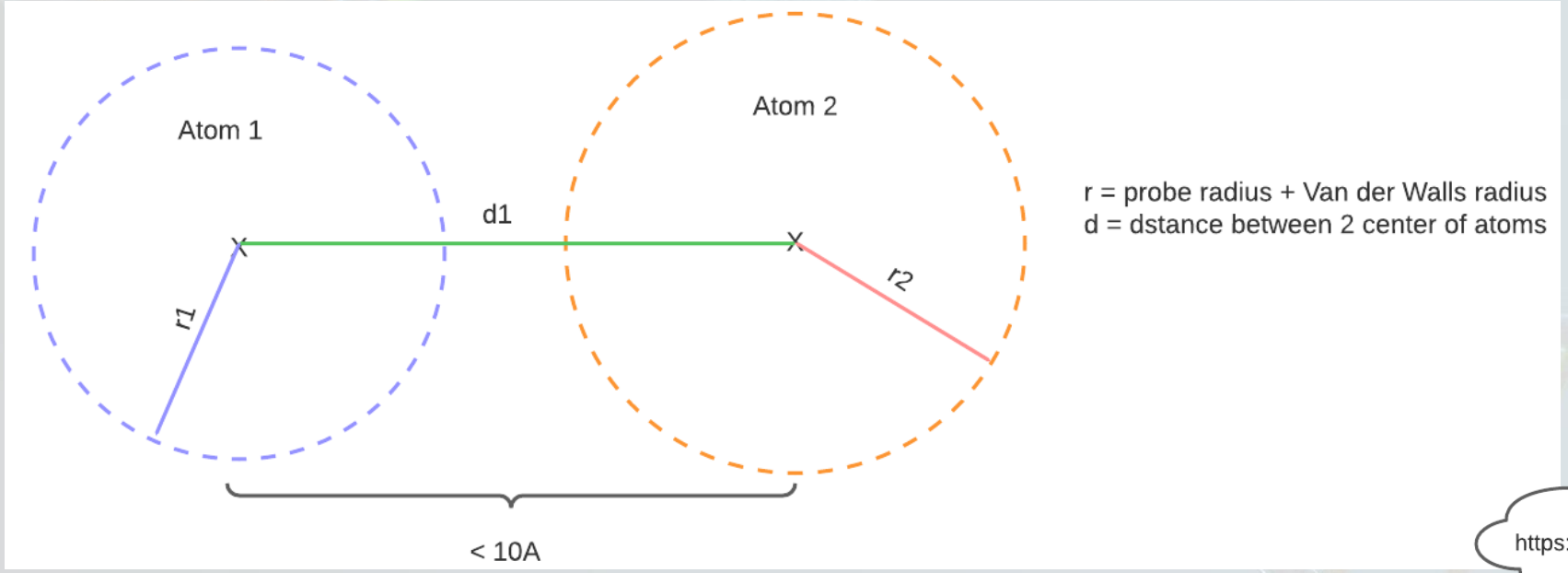
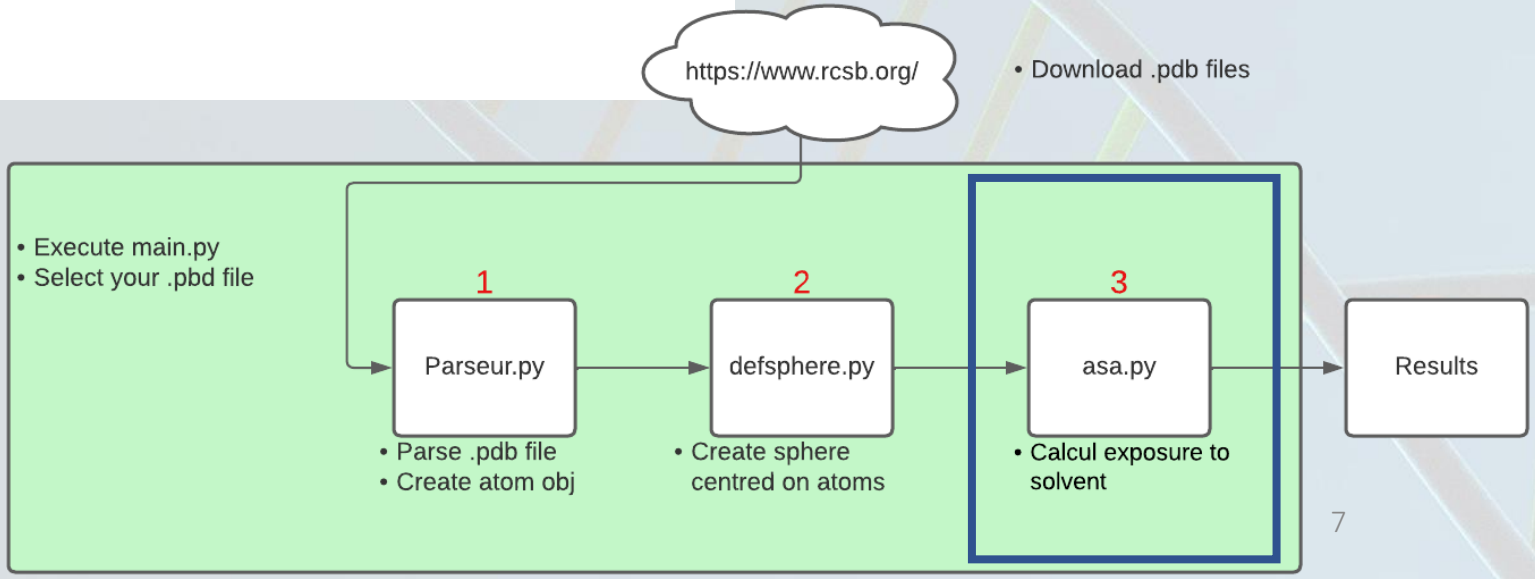
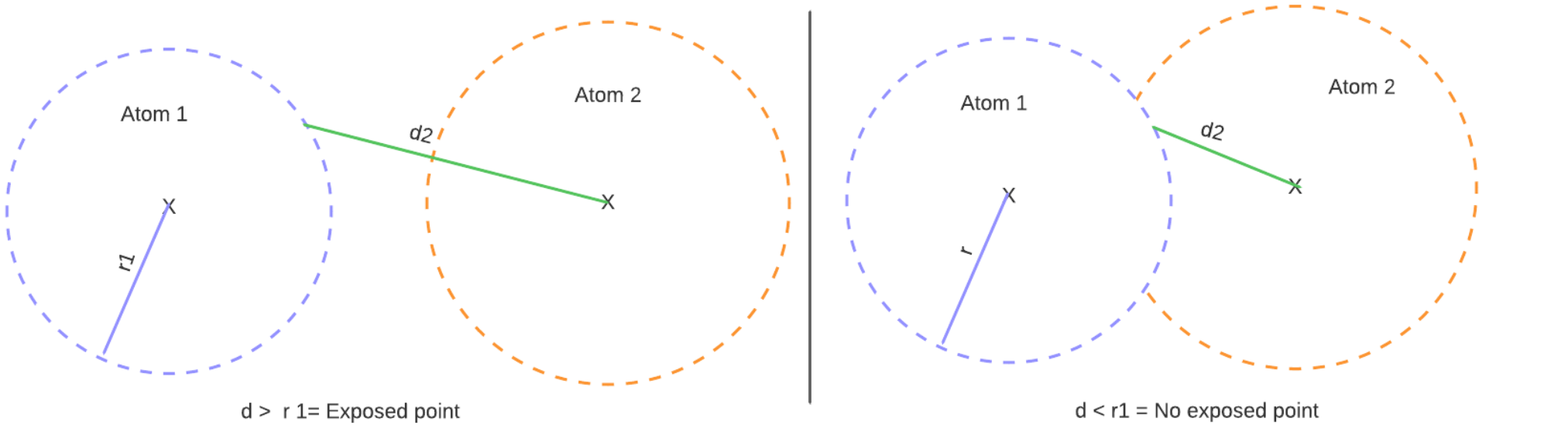
Calcul of ASA



r = probe radius + Van der Walls radius
d = dstance between 2 center of atoms



Calcul of ASA



r 1= probe radius + Van der Walls radius of the first atom
d2 = dstance between first spher and second center

$$ASA = \frac{Sum\ (Exposed\ point)}{Total\ of\ points} * Atom\ Surface$$

Results

- *By residue*
  - Accessible Surface Area (ASA)
  - Relative accessible Surface Area (RSA)
- *All protein*
  - Percentage of accessibility to the solvent
  - Accessible Surface Area (ASA)
  - Relative accessible Surface Area (RSA)

```
id residue:(90, 'ASN')   - asa_abs (Å**2):81.20060872635044    - asa_rel :0.41641337808384843
id residue:(91, 'ALA')   - asa_abs (Å**2):10.337205740159808   - asa_rel :0.08013337783069618
id residue:(92, 'PRO')   - asa_abs (Å**2):53.81821397569194    - asa_rel :0.3384793331804524
id residue:(93, 'GLU')   - asa_abs (Å**2):224.0515585047771    - asa_rel :1.0047155089900317
id residue:(94, 'LEU')   - asa_abs (Å**2):42.69561007213468    - asa_rel :0.2124159705081327
id residue:(95, 'LEU')   - asa_abs (Å**2):1.312639365260779    - asa_rel :0.00653054410577502
id residue:(96, 'LYS')   - asa_abs (Å**2):215.96400628655752   - asa_rel :0.9151017215532098

Le poucentage d'accessibilité est de: 5.9437772667720195
La surface accessible au solvant est de 9617.304319950308Å**2
La surface accessible relative au solvant est de 50.69615441413572%
```

Results

Files	Atoms	Results program A**2	Results DSSP A**2	Differences
1bja.pdb	1423	9617.3	9721.4	-1.0%
1bjb.pdb	431	2450.5	2431.1	0.8%
1bjj.pdb	5837	37862.7	37435.6	1.1%
1bzv.pdb	362	3704.4	3839.8	-3.5%
1jhg.pdb	1806	8133.5	8222.1	1.0%
2ml6.pdb	2354	9958.1	10266.5	3.0%
6a5j.pdb	260	1596.43	1556.6	2.6%

MERCI

References

[1] Lee, B; Richards, FM. (1971). "The interpretation of protein structures: estimation of static accessibility" . J Mol Biol. 55 (3): 379–400. doi:10.1016/0022-2836(71)90324-X.

[2] https://www.rcsb.org/

[3] 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.

[4] Tien, et al.. (2013). "Maximum allowed solvent accessibilites of residues in proteins". PLOS ONE. 8 (11): e80635. doi:10.1371/journal.pone.0080635