SOLVENT ACCESSIBLE SURFACE AREA CALCULATION

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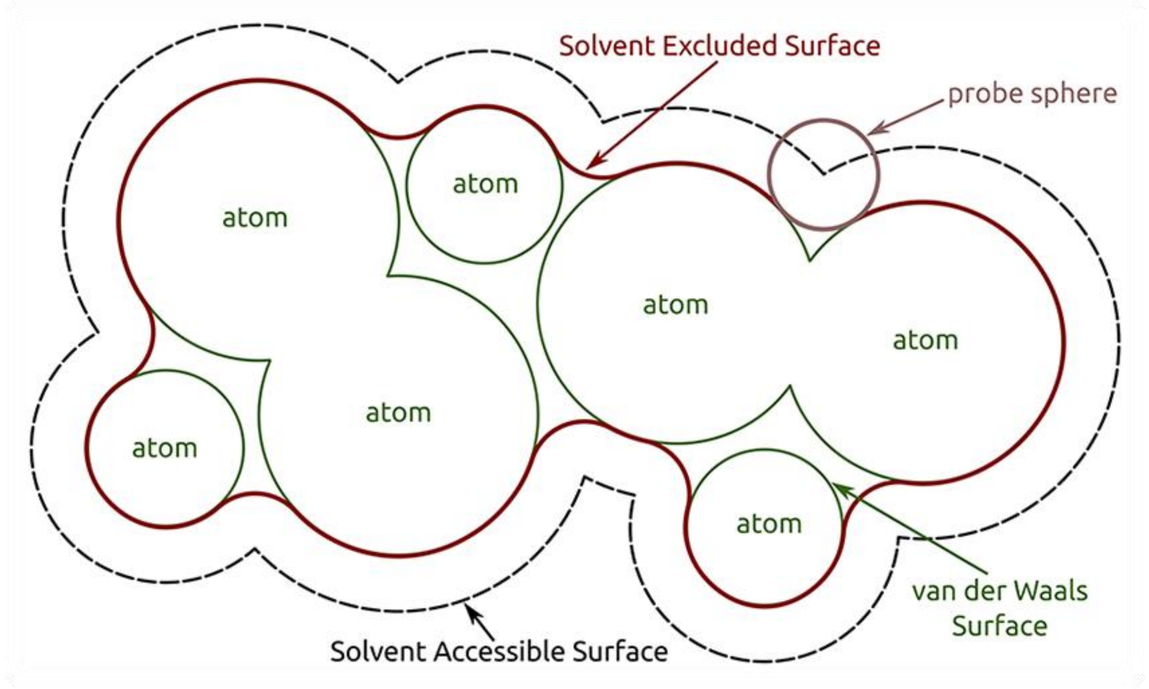
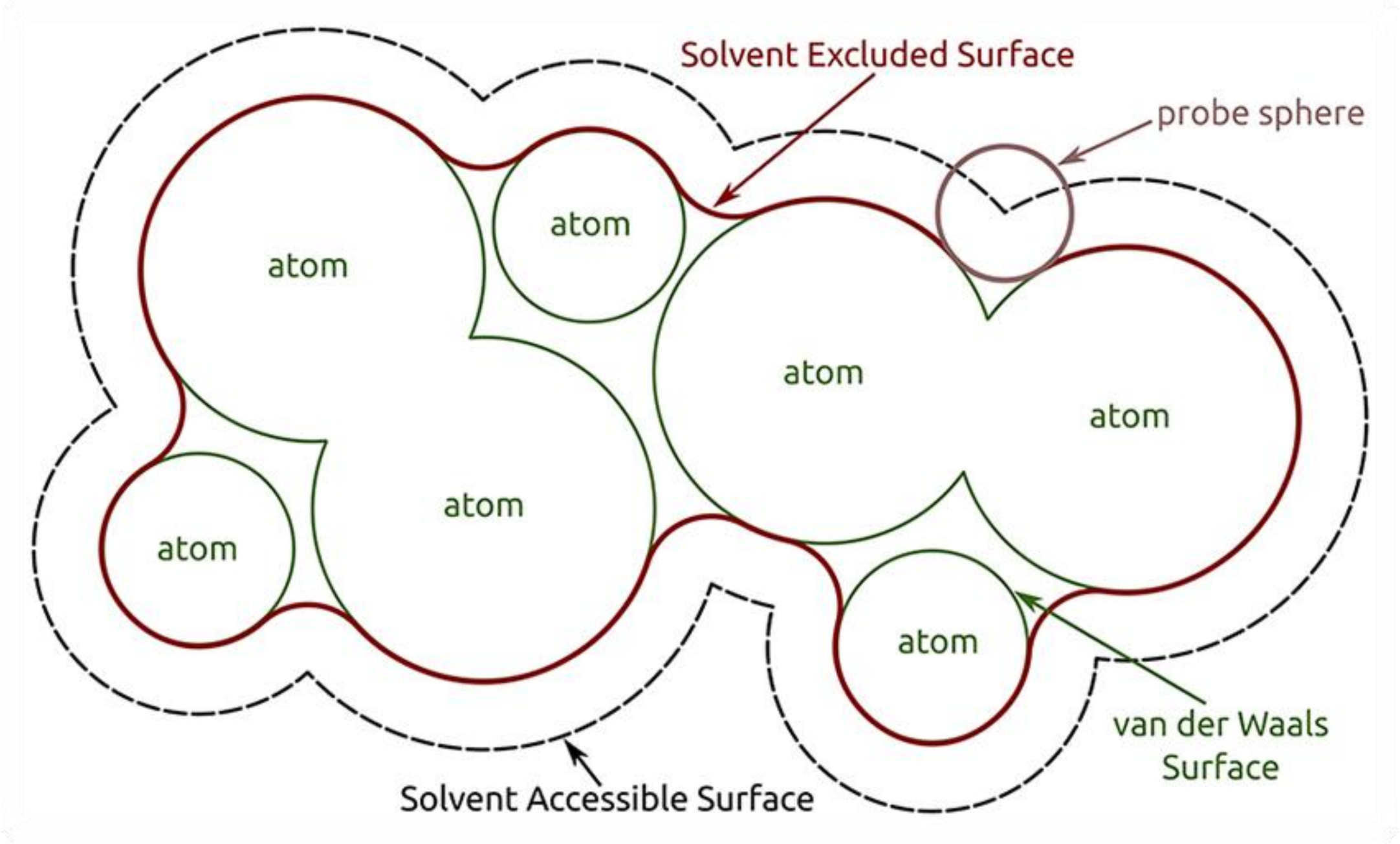
SOLVENT ACCESSIBLE SURFACE AREA

(SASA)

Area around a protein defined by the centre of a hypothetical solvent sphere that corresponds to the van der Waals contact surface of the molecule




Solvent Excluded Surface
probe sphere
atom
atom
atom
atom
atom
atom
atom
van der Waals
Surface
Solvent Accessible Surface

CODE USAGE

Terminal

```
❯ python src/SASA_calc.py
usage: SASA_calc.py [-h] [--model MODEL] [--points POINTS] [--probe PROBE]
[--output {residue,atomic,total,complete}] pdb_file
```

CODE OUTPUT EXAMPLE

output_example

```
...
ATOM    2949   OD1  ASP     B  172       0.00
ATOM    2950   OD2  ASP     B  172      20.36
...
RES                 PHE     B  173     103.86      45.55
RES                 TYR     B  174     198.86      77.98
CHAIN                       A         8663.91   4389.16
CHAIN                       B         8557.98   4323.19
TOTAL                               17221.89   8712.35
```

SASA VALUES COMPARISON WITH NACCESS

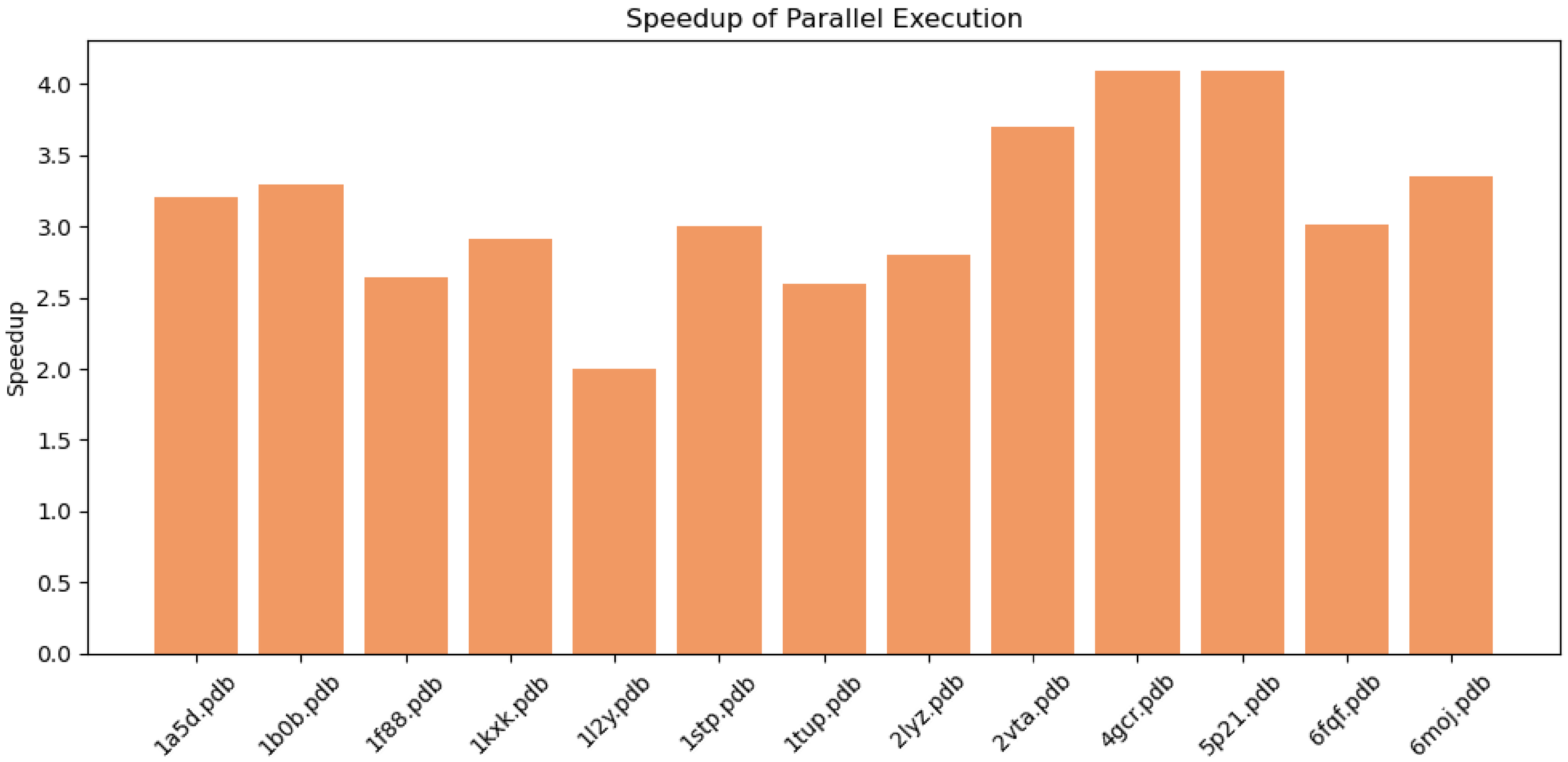
NACCESS comparison

PDB ID	NACCESS	CUSTOM	ERROR (%)
2vta	13929.90	14088.89	1.14
1f88	27522.30	28669.05	4.17
5p21	8505.90	8384.93	1.42
1b0b	6929.50	6883.62	0.66
1kxk	12442.90	12725.68	2.27
6moj	20176.80	20920.29	3.68
6fqf	24588.70	24092.77	2.02
4gcr	8802.00	8870.93	0.78
1a5d	17094.00	17221.89	0.75
2lyz	6645.80	6692.97	0.71
1tup	32948.50	33401.08	1.37
1stp	7031.10	6881.90	2.12

Average error: 1.76%

Max error: 4.17%, Min error: 0.66%, Std Dev: 1.11%

MULTIPROCESSING IMPLEMENTATION



CONCLUSIONS

Our framework, validated against NACCESS and optimised through multiprocessing, proves to be reliable and efficient