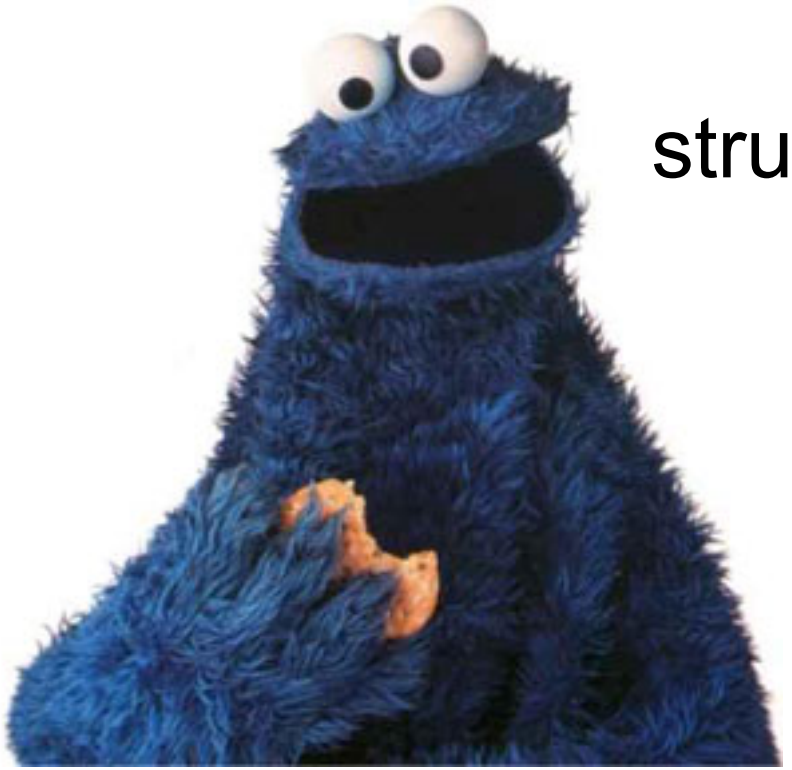
BisKit

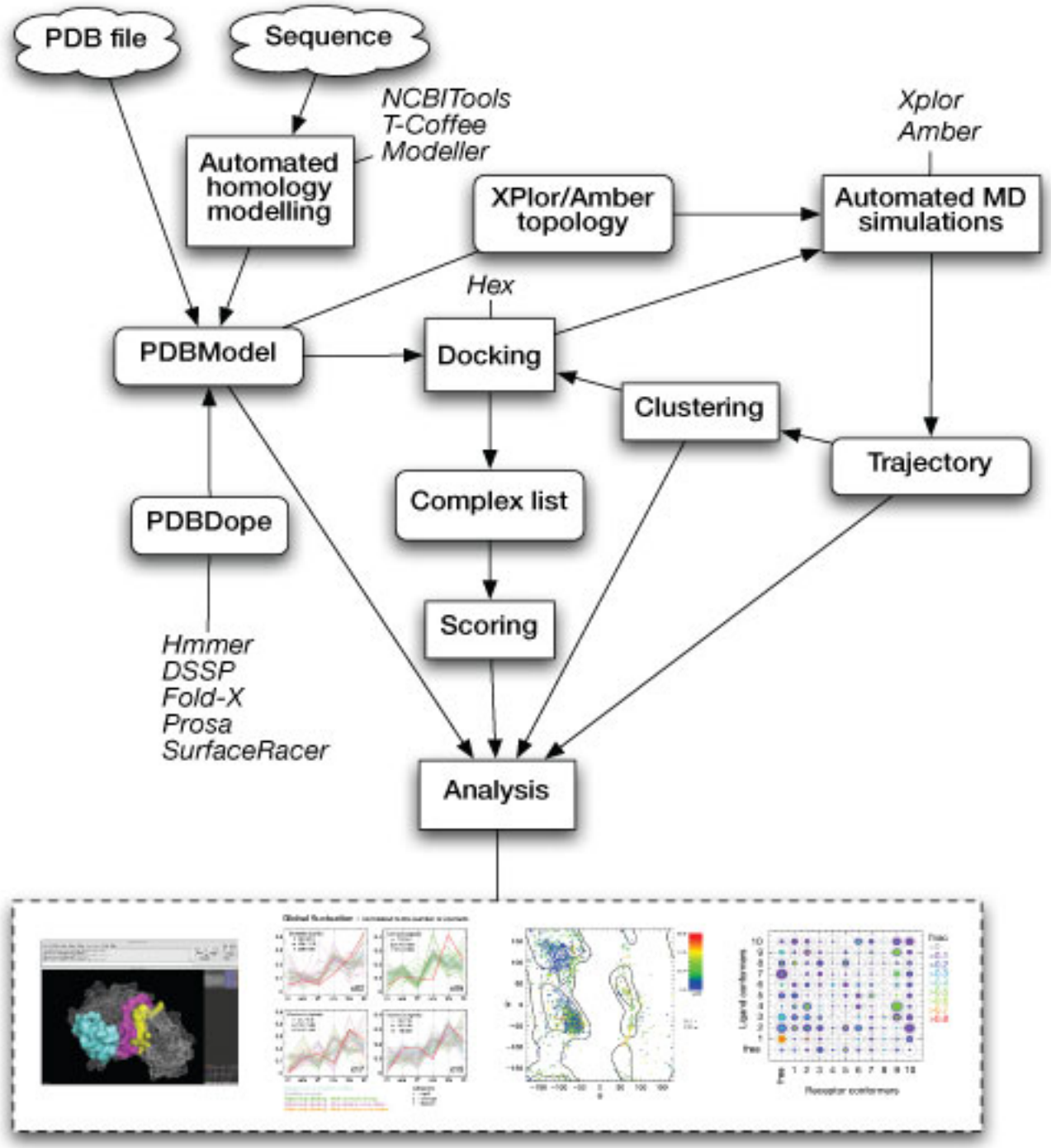


structural bioinformatics made easy
(or at least less painful)

The story of Biskit

Overview

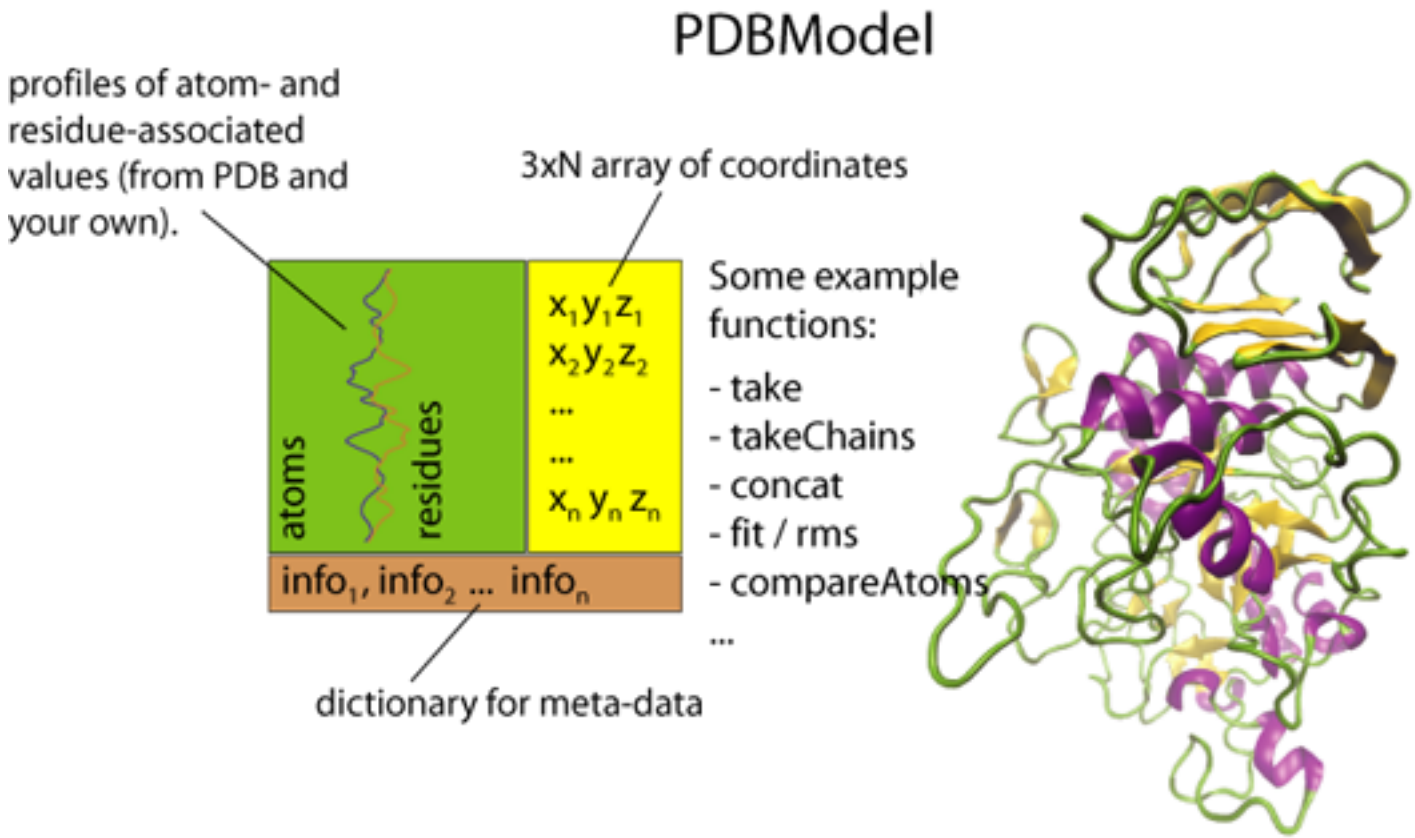
- pythonic handling of ...
  - structures
  - complexes
  - trajectories
  - ...
- efficient number crunching
- wrapping external programs
- data integration
- workflows
- parallelization



Content

1. Handling Structures (PDBModel)
    - load, inspect, associated data (profiles)
    - select, compress, slice, concatenate
    - rms, fitting, comparing
    -
2. Adding data (PDBDope)
    - surface areas, secondary structure, conservation
    -
3. Persistence & Pickling
    -
4. Trajectories
    - Amber tools
    - rms, fluctuations, fitting
    - select, compress, slice, concatenate
    - cluster
    -
5. Advanced topics
    -
6. biskit 3.0

1. Handling Structures



2. Adding Data

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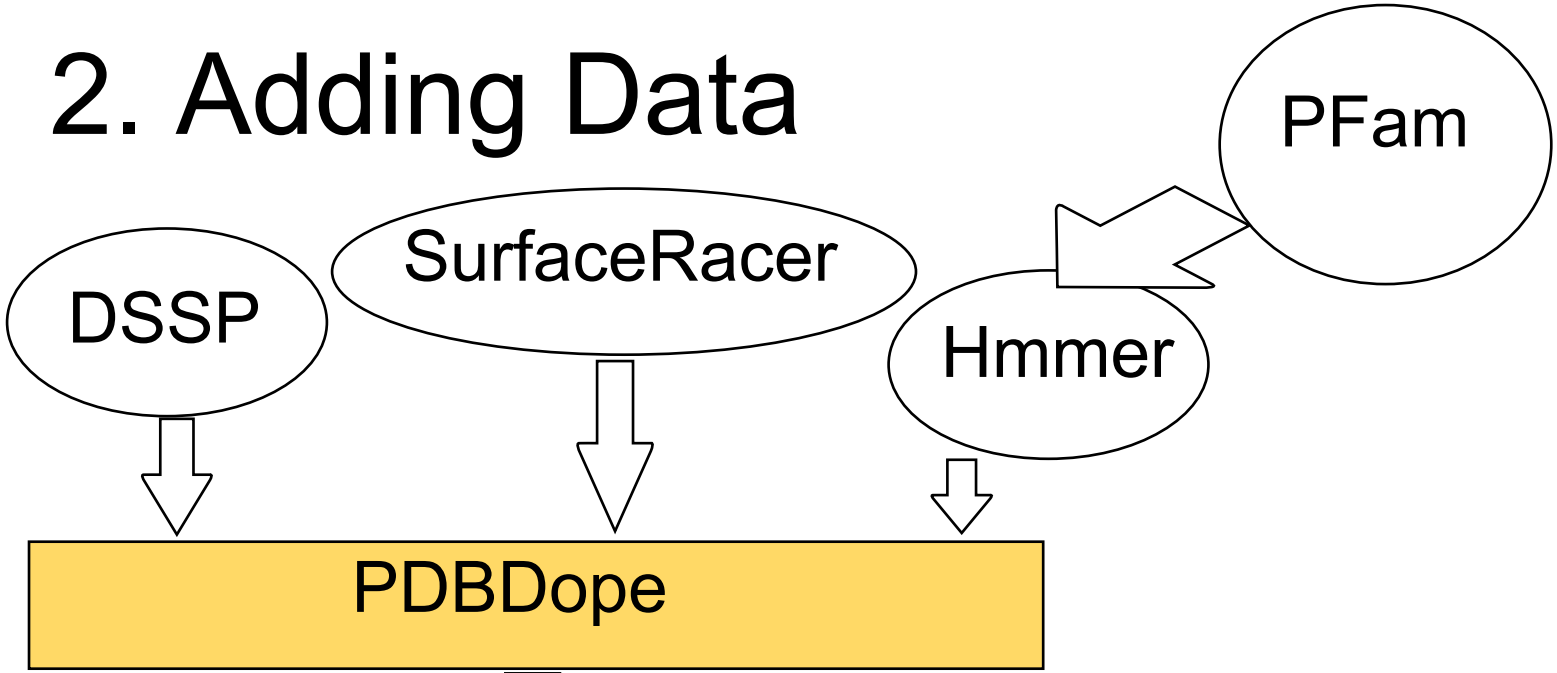
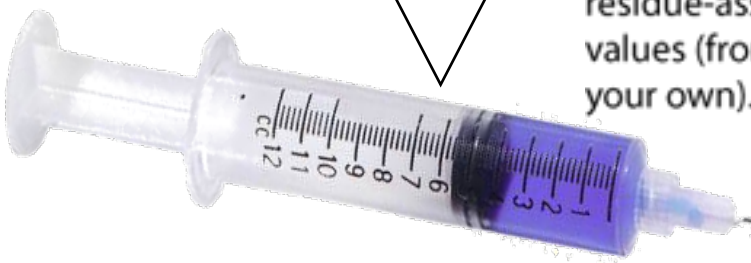
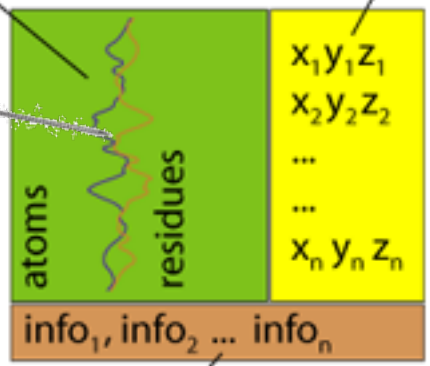




profiles of atom- and residue-associated values (from PDB and your own).

PDBModel

3xN array of coordinates

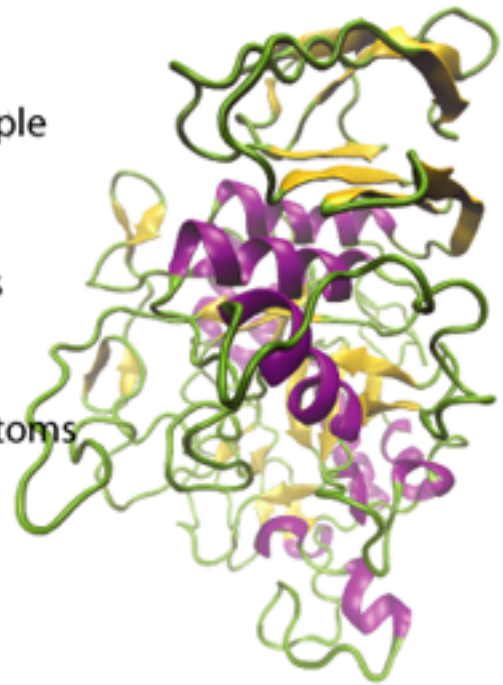


dictionary for meta-data

Some example functions:

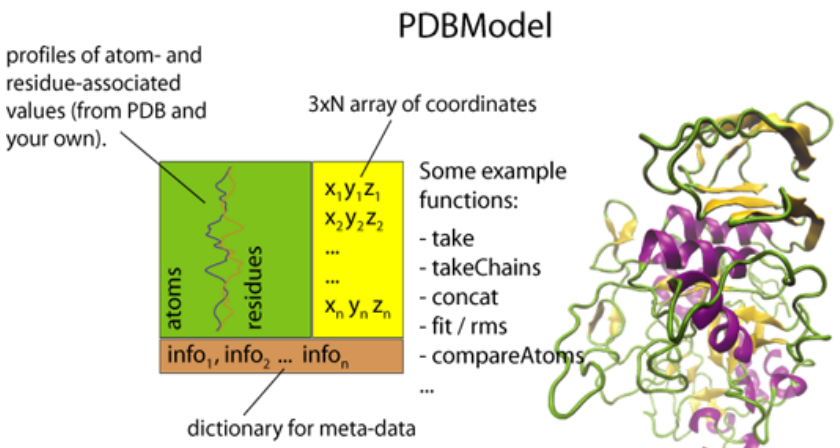
- take
- takeChains
- concat
- fit / rms
- compareAtoms

...



Persistence & Pickling

Persistence & Pickling



dump

saveAs

load

4. Trajectories

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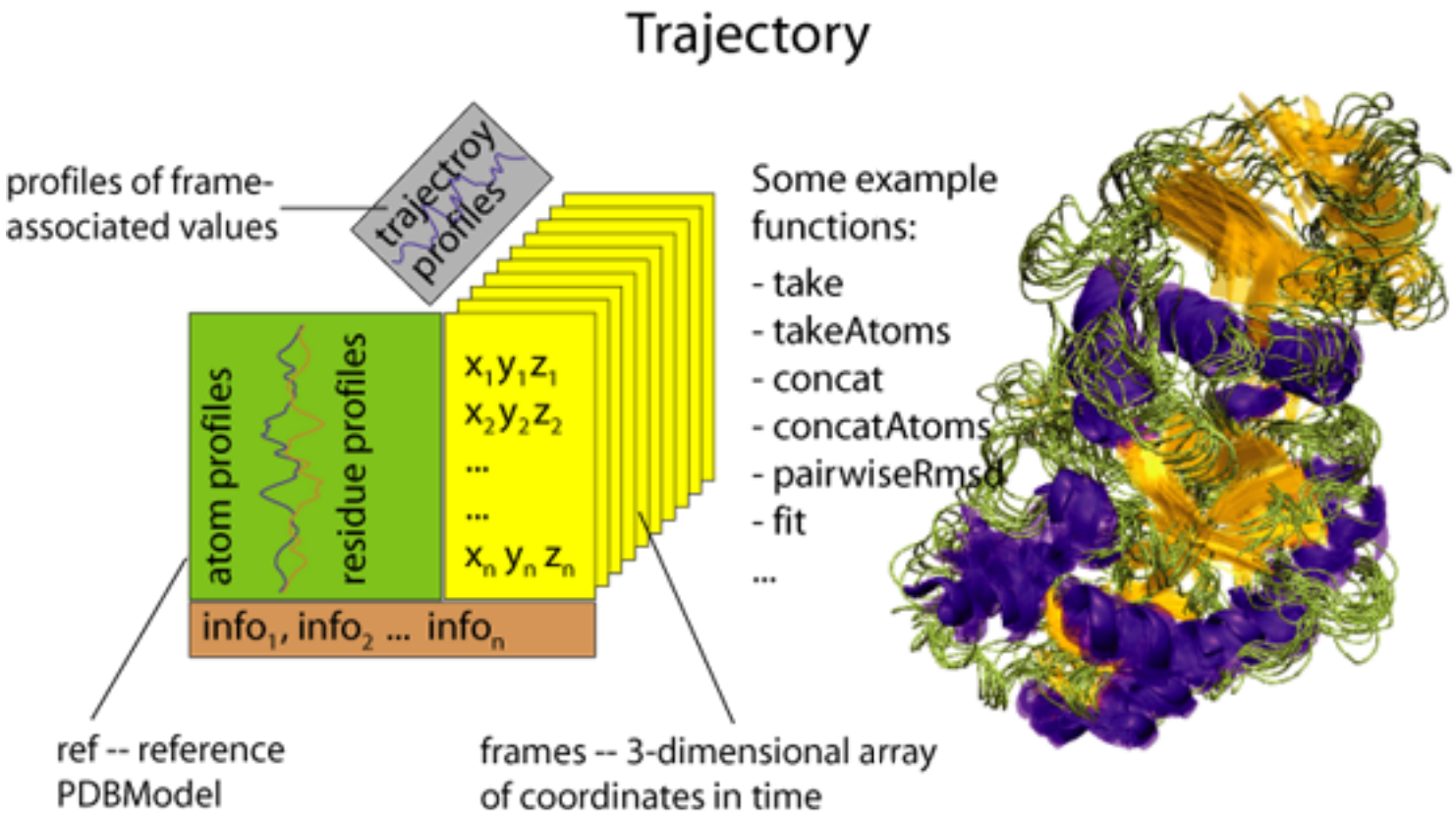
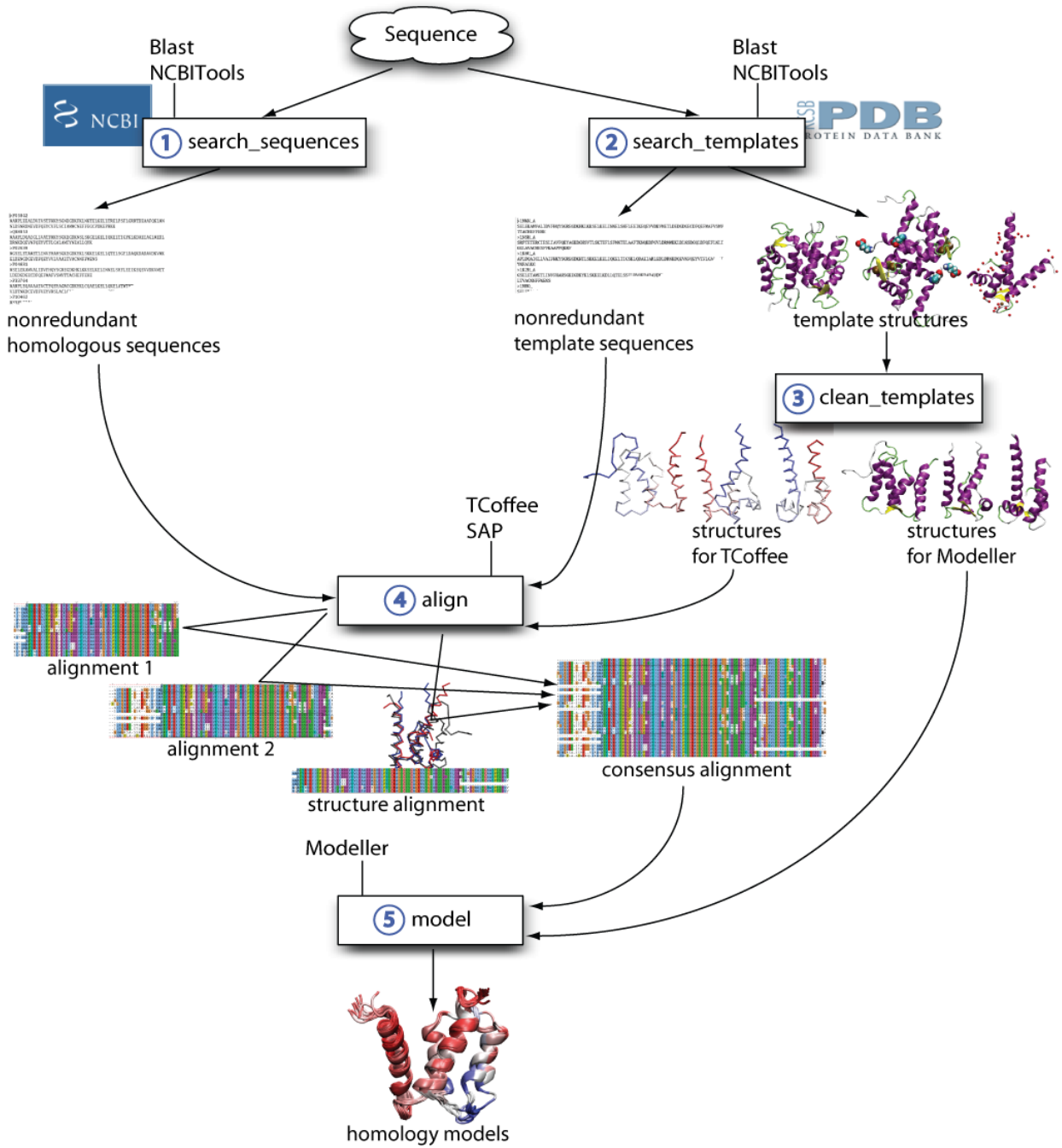


Advanced Topics

- Protein-Protein Complexes and Docking
- Homology Modeling

Automatic Homology Modeling



biskit 3.0

- Biskit -> biskit
- python 3.0 compatibility
- setup.py installer
- use python Properties
- usability -- your feedback!
- documentation -- your feedback!