Ab initio tutorial (part II)

- Ambimeter
  - model independent ambiguity score
- Damclust
  - alternative to Damaver
- Gasbor (local & online)
  - real/reciprocal space
- Monsa (online)
  - Nucleoprotein
  - Dimeric complex
- Dammin
  - limited search volume
  - anisometry restraint
AMBIMETER: tool for Ambiguity Assessment

Map of renormalized scattering profiles from exhaustive set of shape topologies is employed to quantitatively evaluate the ambiguity of a small-angle-scattering curve.

AMBIMETER is now a part of SASFLOW pipeline

18 Skeletons with identical SAXS curves
DamClust: Assessment of multimodality

(has damaver & friends inside)

Clustering of multiple SAS models

- Discrepancies (distances) between multiple models as criteria for grouping
- Normalized spatial deviation serves as a distance between heterogeneous models (e.g. bead models)
- \textit{R.m.s.d}. is employed for those with atom-to-atom correspondence (e.g. rigid body models)

Creates the complete graph by iteratively joining the clusters (singles)

Selects the optimal threshold as a compromise between the number of clusters and averaged spread within the cluster
Dummy Residues Model

- Proteins typically consist of folded polypeptide chains composed of amino acid residues
- At a resolution of 0.5 nm each amino acid can be represented as one entity (dummy residue)
- In GASBOR a protein is represented by an ensemble of $K$ DRs those are
  - Identical
  - Have no ordinal number
  - For simplicity are centered at the $C_\alpha$ positions
$\rho = 0.334 \text{ e/Å}^3$

$\Delta \rho = 0.03 \text{ e/Å}^3$

Width = 3Å

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MONSA (multiphase modelling)

1. 1 phase = 1 component of a complex particle
2. For each phase, Rg, V and its scattering curve can be given
3. For each curve, contrast of each phase are specified

contrast variation and/or use of partial constructs
Monsa case 1: protein-RNA complex

252 AA protein (two domains)
67 nucleotides RNA

Three curves in total:
Free RNA
Complex
Free protein
Monsa case2: dimeric complex

- 172 AA (20kDa) and 538 AA (70 kDa) proteins
- Dimerization via small one
- Two-fold symmetry axis
Dammin features missing in Dammif

- Specific (limited) search volume (sphere, ellipsoid, cylinder, parallelepiped, User supplied)
- Icosahedral and cubic symmetries
- Anisometry restraint
**Anisometry (direction)**

- both shapes are symmetric and extended