New Developments in ATSAS 3.0

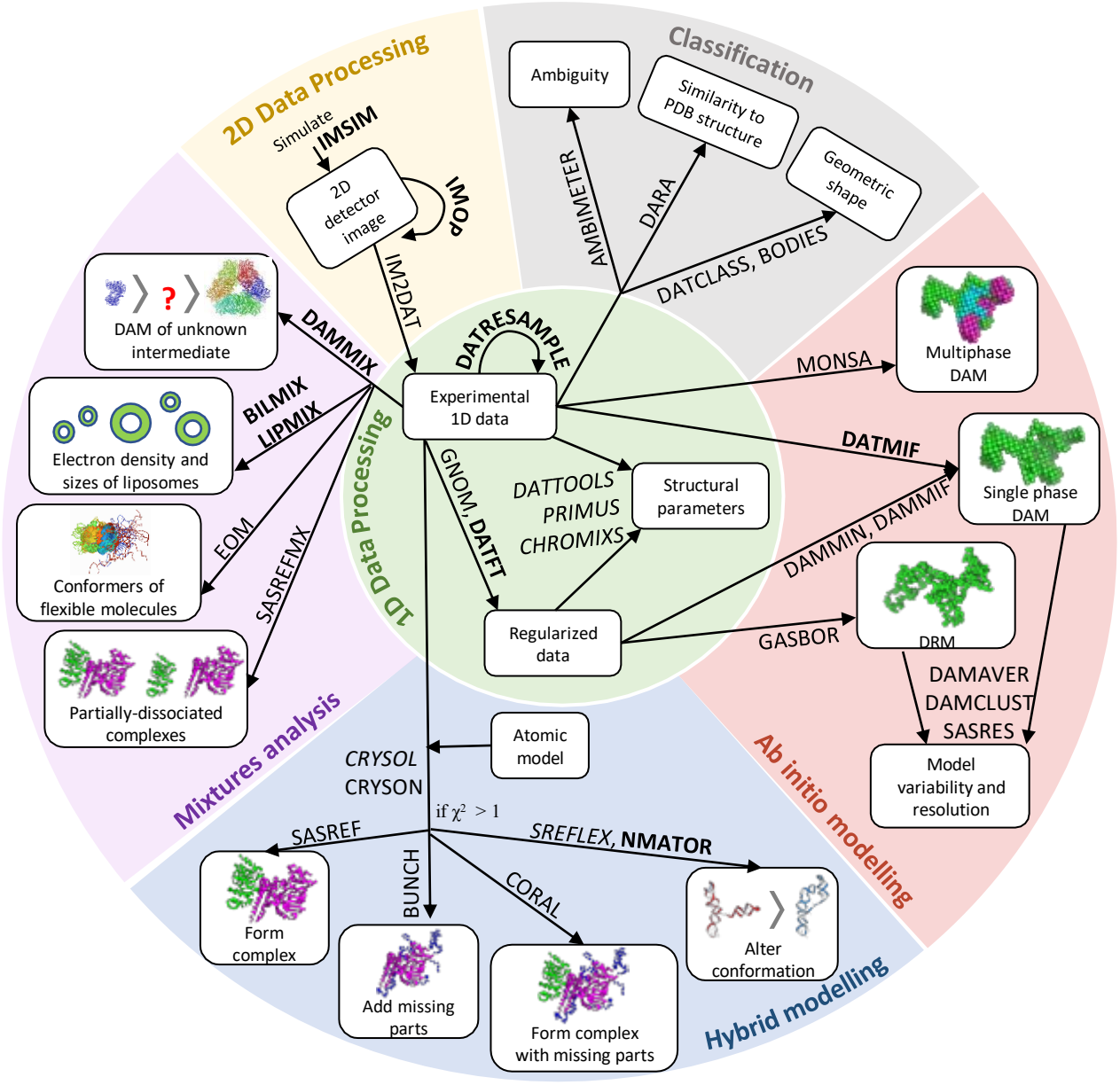
Karen Manalastas-Cantos

P12 Virtual User Meeting

17 Nov 2020

ATSAS

- processing, visualization, analysis and modelling of small-angle scattering data



Manalastas-Cantos et al. ATSAS 3.0 (accepted) JAC

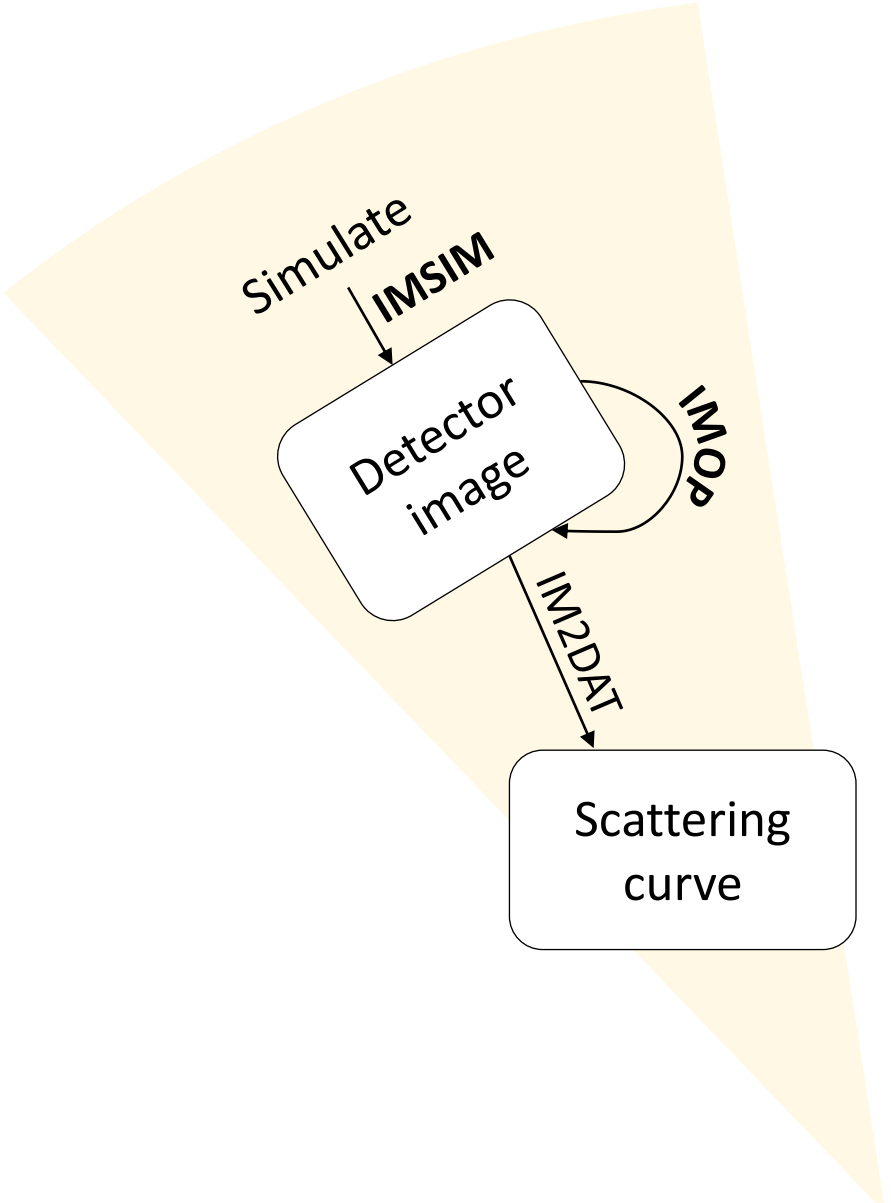
2D data processing

IM2DAT (formerly RADAVER)

- Azimuthal/radial averaging of 2D detector image into 1D scattering curve

New programs

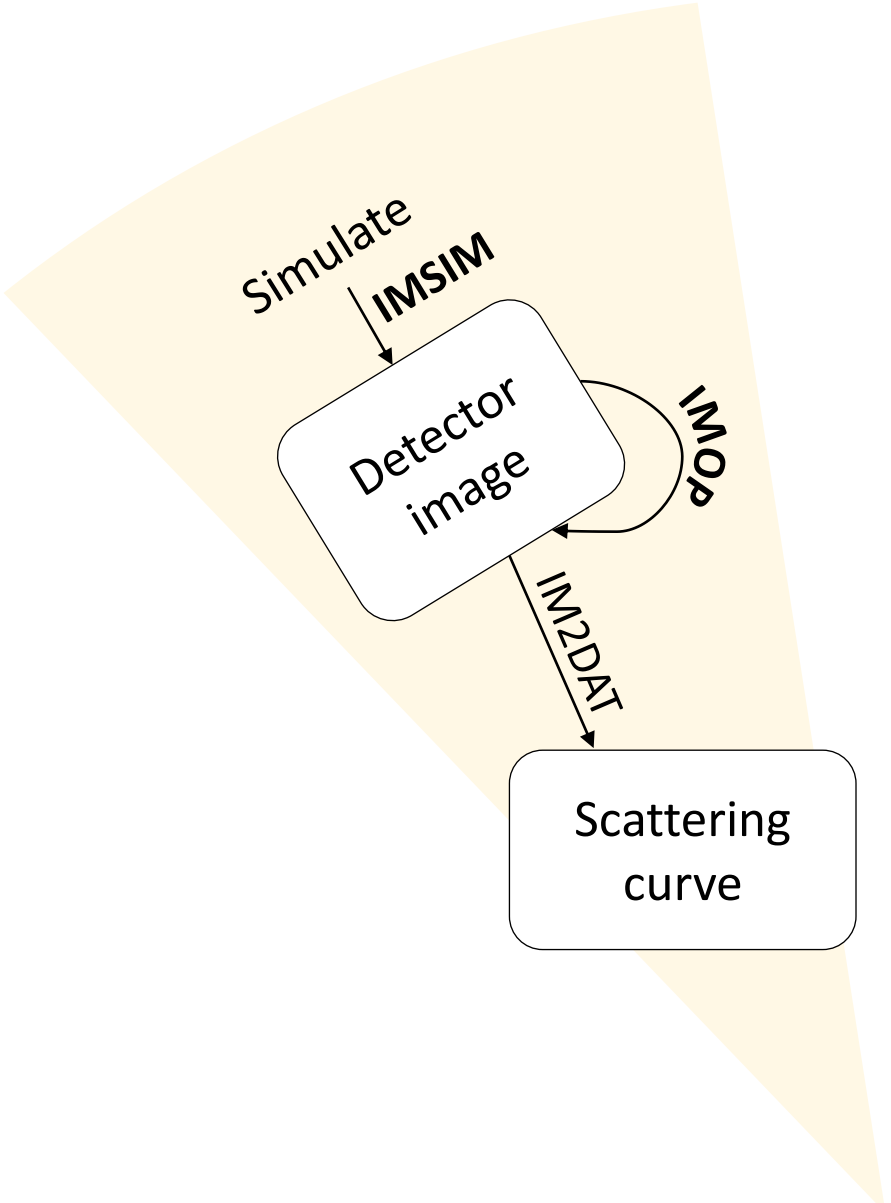
- IMOP
- IMSIM



2D data processing

IMOP (**IM**age **OP**erations)

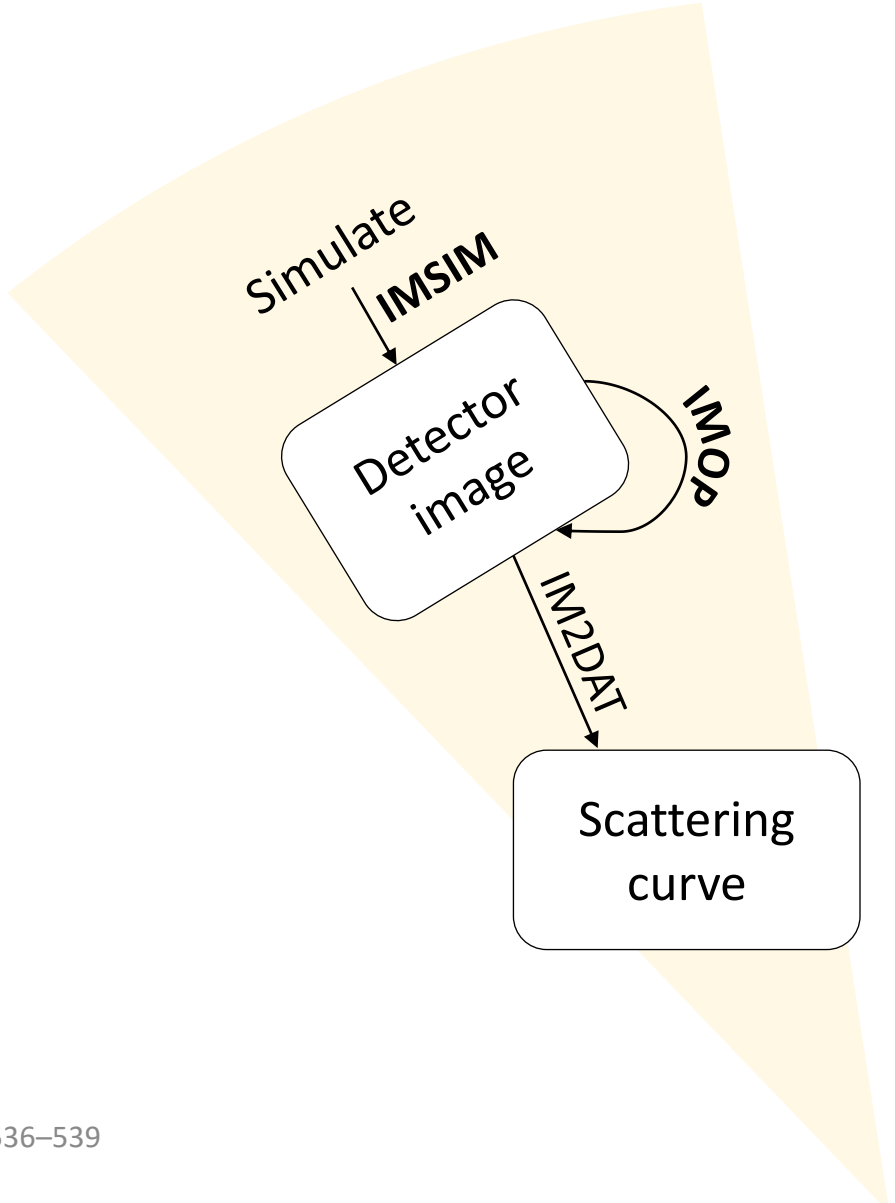
- Does operations on 2D images of equal size
  - Operators: ADD, SUB, AND, OR, XOR
- Application:
  - Applying a mask to a detector image
  - Validating 1D operations



2D data processing

IMSIM (**IM**age **SIM**ulation)

- Simulates 2D SAXS patterns
  - Intensities and errors have same statistical properties as actual experimental data
  - Incorporates experimental parameters (solute concentration, detector, detector distance, wavelength, etc.)
- Applications:
  - To generate large, benchmarking datasets
  - For beamline setup
- Usage:
  - Input: .abs file from CRYSOL and experimental parameters
  - Example run in IMSIM manual



Franke, Hajizadeh & Svergun (2020) JAC. 53, 536–539

CRYSOL for anomalous scattering

CRYSOL: evaluates scattering from atomic structures

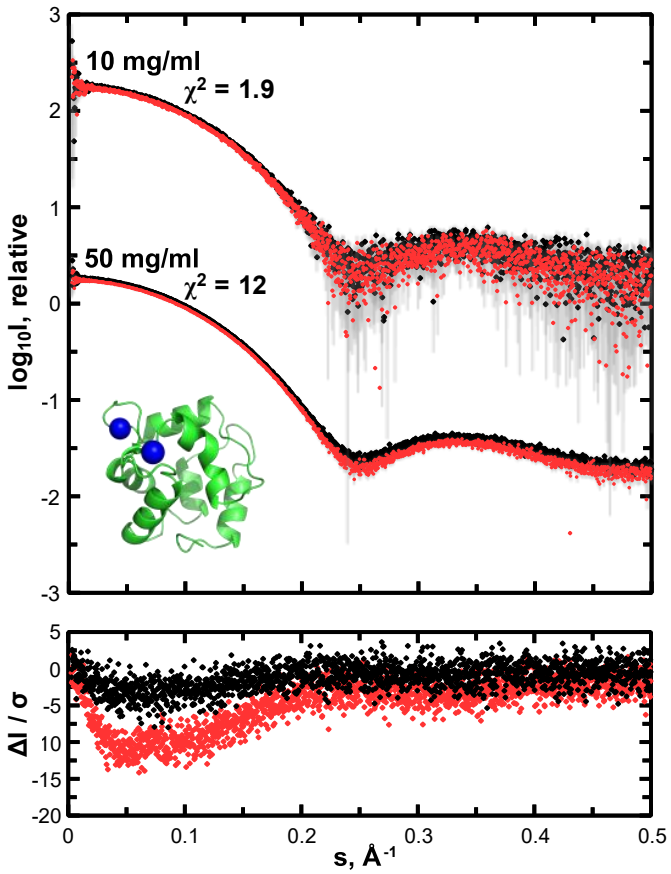
Anomalous scattering

- absorption events occurring at wavelengths near an atom's absorption edge
- can be used to extract distances between absorbing atoms

Usage:

crysol -en <incoming energy in eV> -el <element name> <PDB file>

CRYSOL → IMSIM → IM2DAT



default
anomalous

10 mg/ml
50 mg/ml

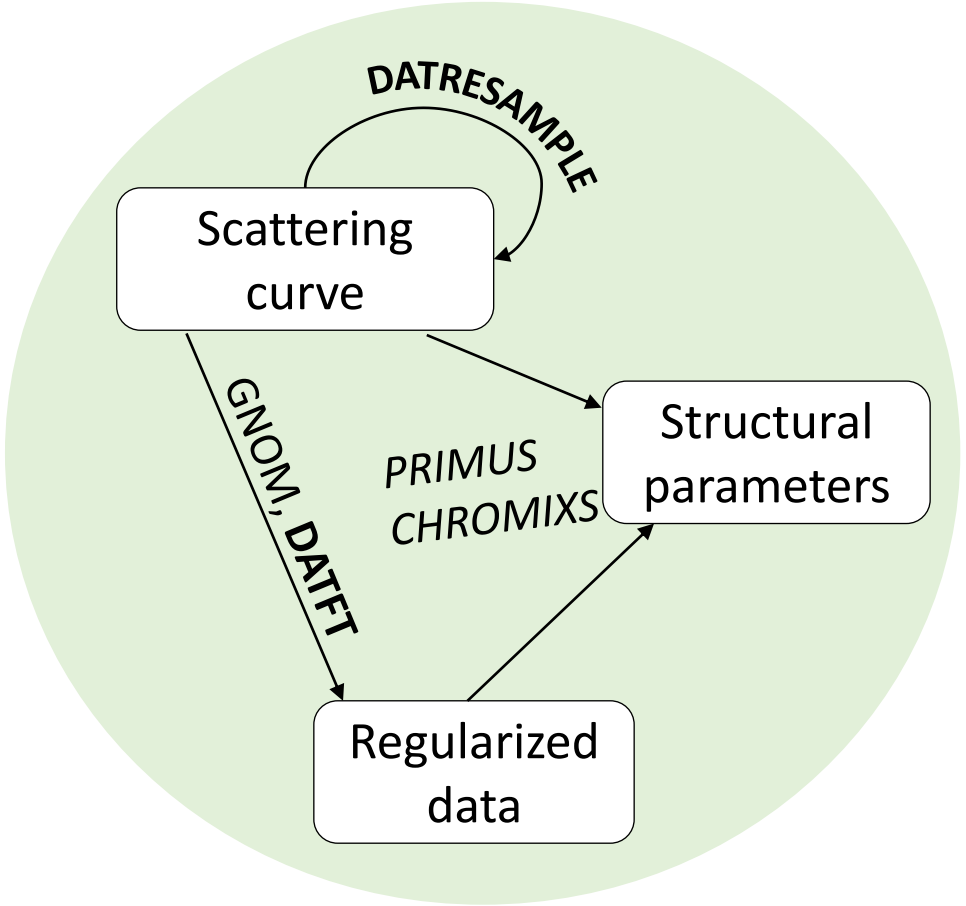
Tools for scattering curves

GUI updates

- CHROMIXS
- PRIMUS

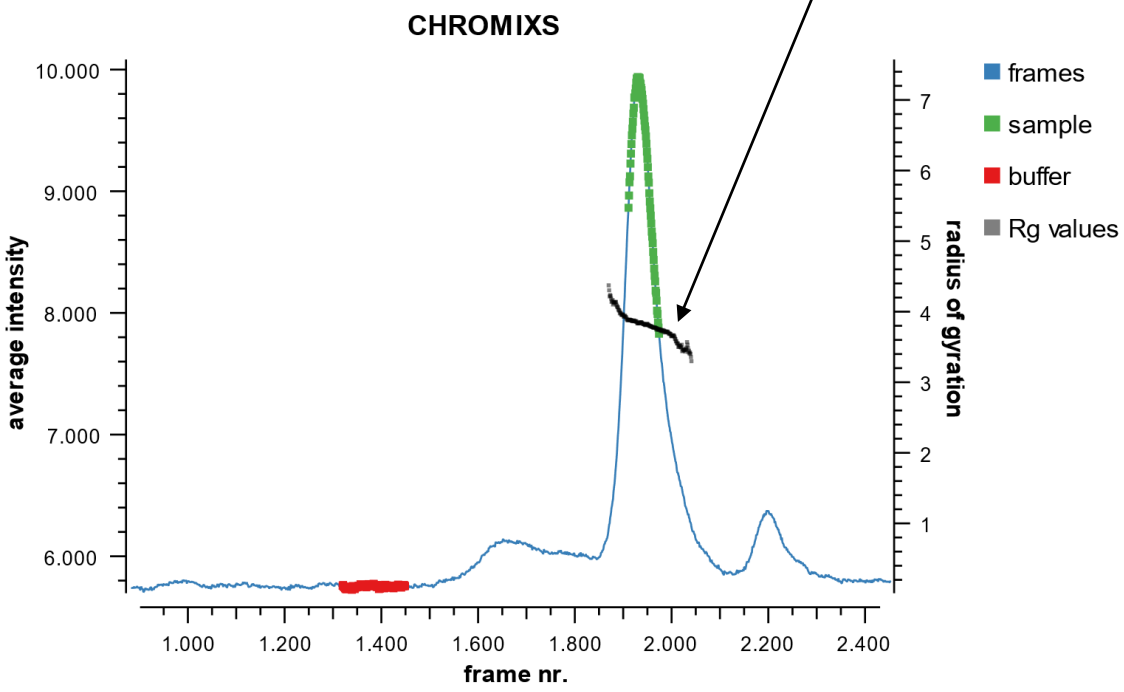
New programs

- DATRESAMPLE
- DATFT

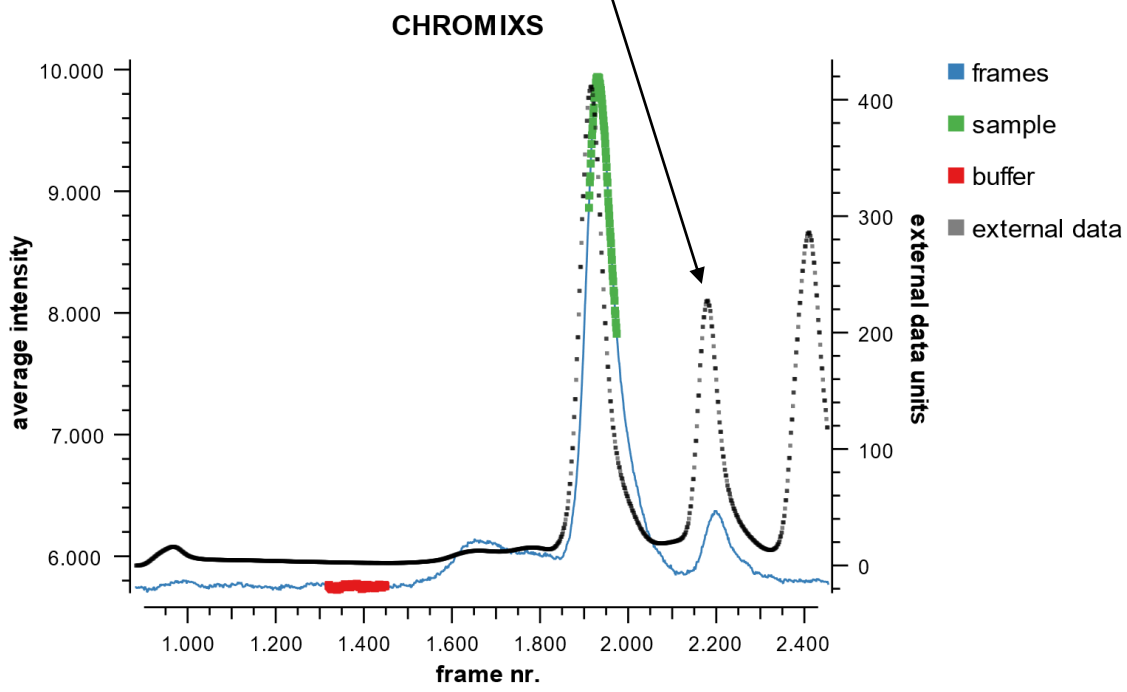


GUI updates: CHROMIXS

(1) Calculate Rg or MW
for selected set of frames



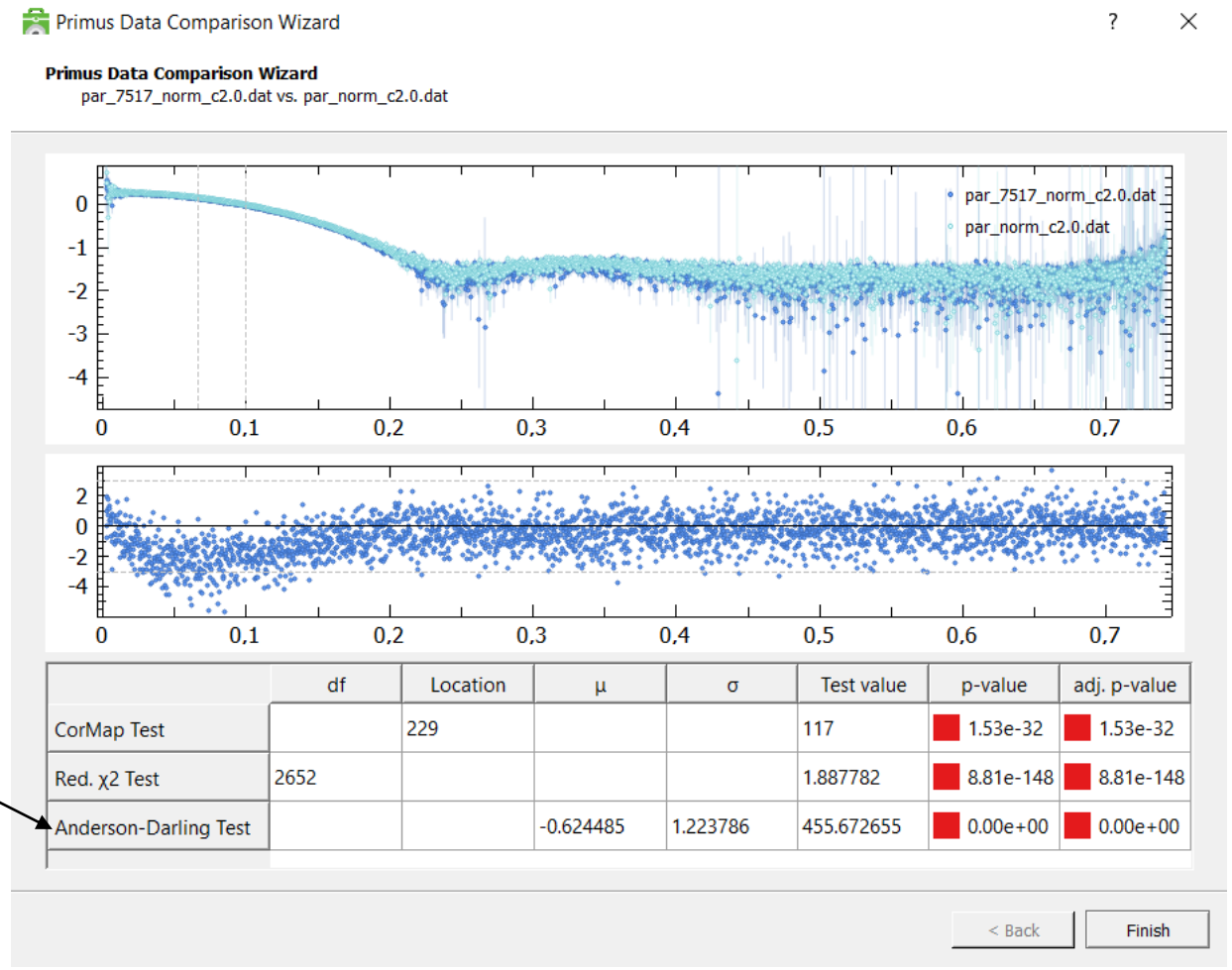
(2) Load complementary time
course data (e.g. UV absorbance)



Panjkovich & Svergun (2018) Bioinformatics. 34(11), 1944-1946

GUI updates: PRIMUS

- Updated to Qt5
  - Improved display
  - Configurable graphics export
- Added data comparison test (Anderson-Darling)

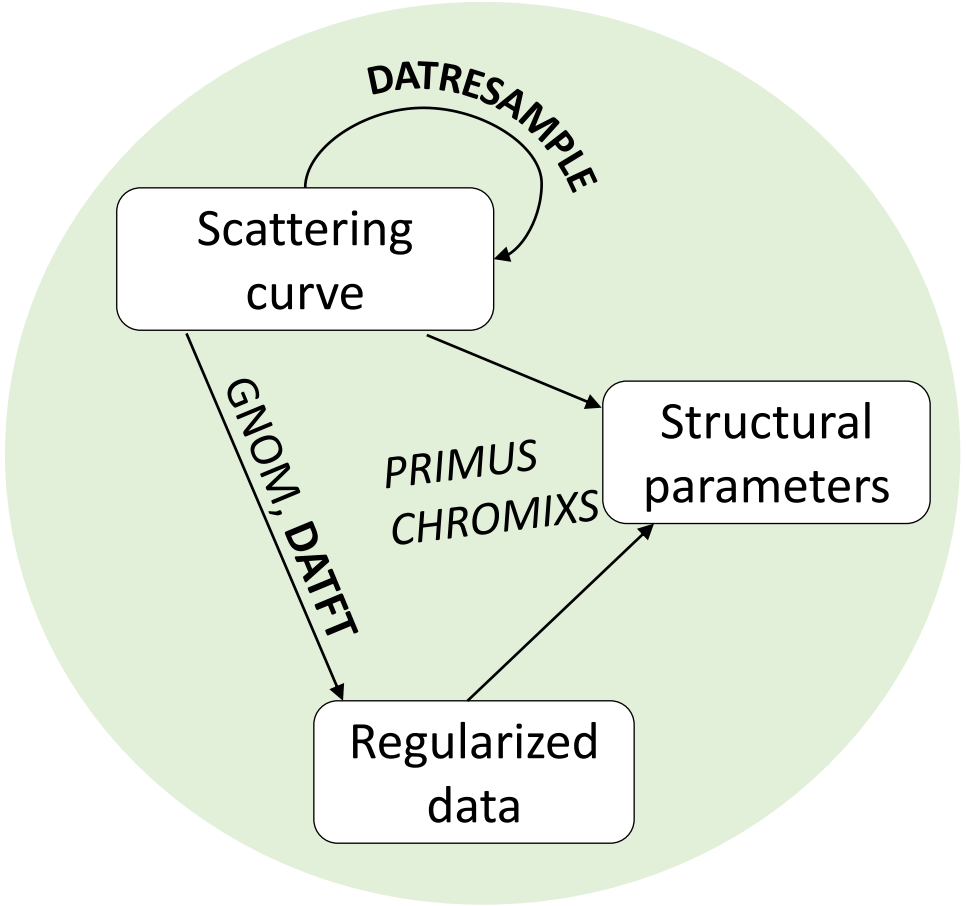


New tools for scattering curves

DATRESAMPLE

- From a single scattering curve, randomly resamples additional scattering curves representing the same sample

- Applications
  - Resampled scattering curves can be used to estimate variance of point estimates (e.g. D_{max}, V_p)
  - To generate a large benchmark dataset



New tools for scattering curves

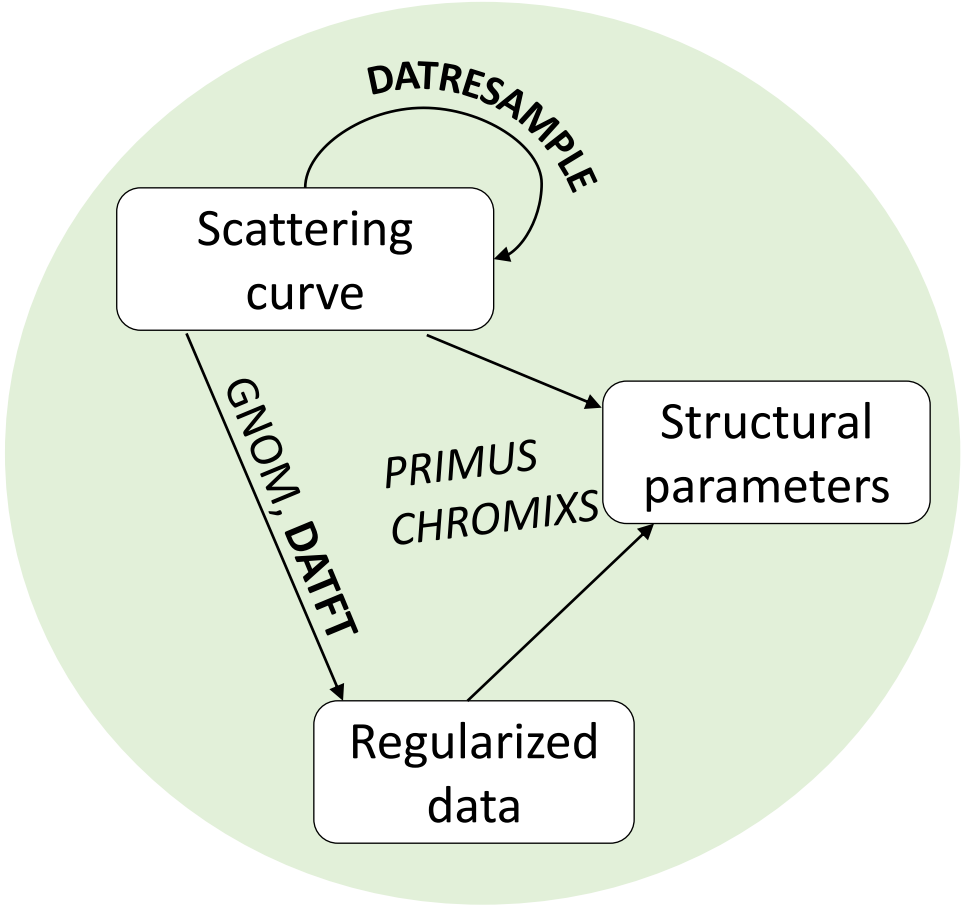
DATFT

- Computes $P(r)$ through direct Fourier transform

$$P(r) = \frac{r}{2\pi^2}\int_0^\infty sI(s)\sin(sr)\,ds$$

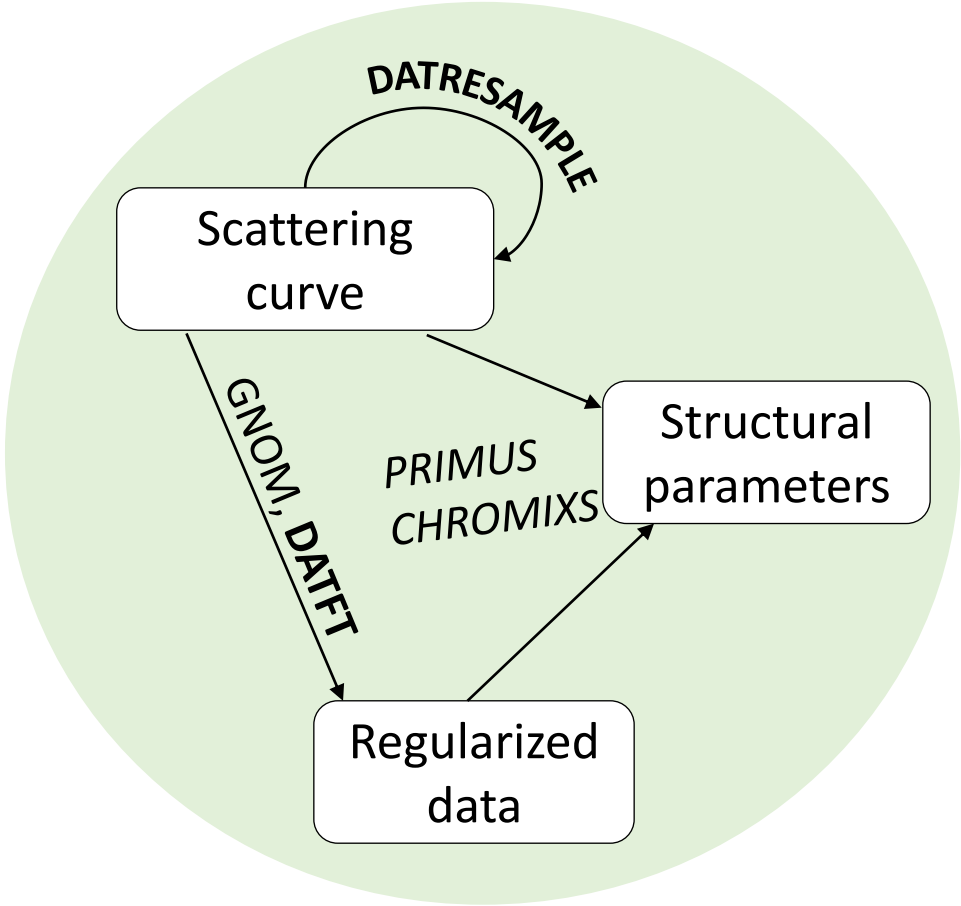
where at high s, $I(s) = s^{-4}$

- Use case
  - Low-noise experimental data on equidistant s grid.



New tools for scattering curves

- Auxiliary tools
  - **PDDFFIT**
    - determines whether $P(r)$ is consistent with the experimental data
  - **OUT2POFR**
    - extracts $P(r)$ from GNOM .out file
  - **OUT2FIT**
    - extracts fit between experimental and regularized data from GNOM .out file



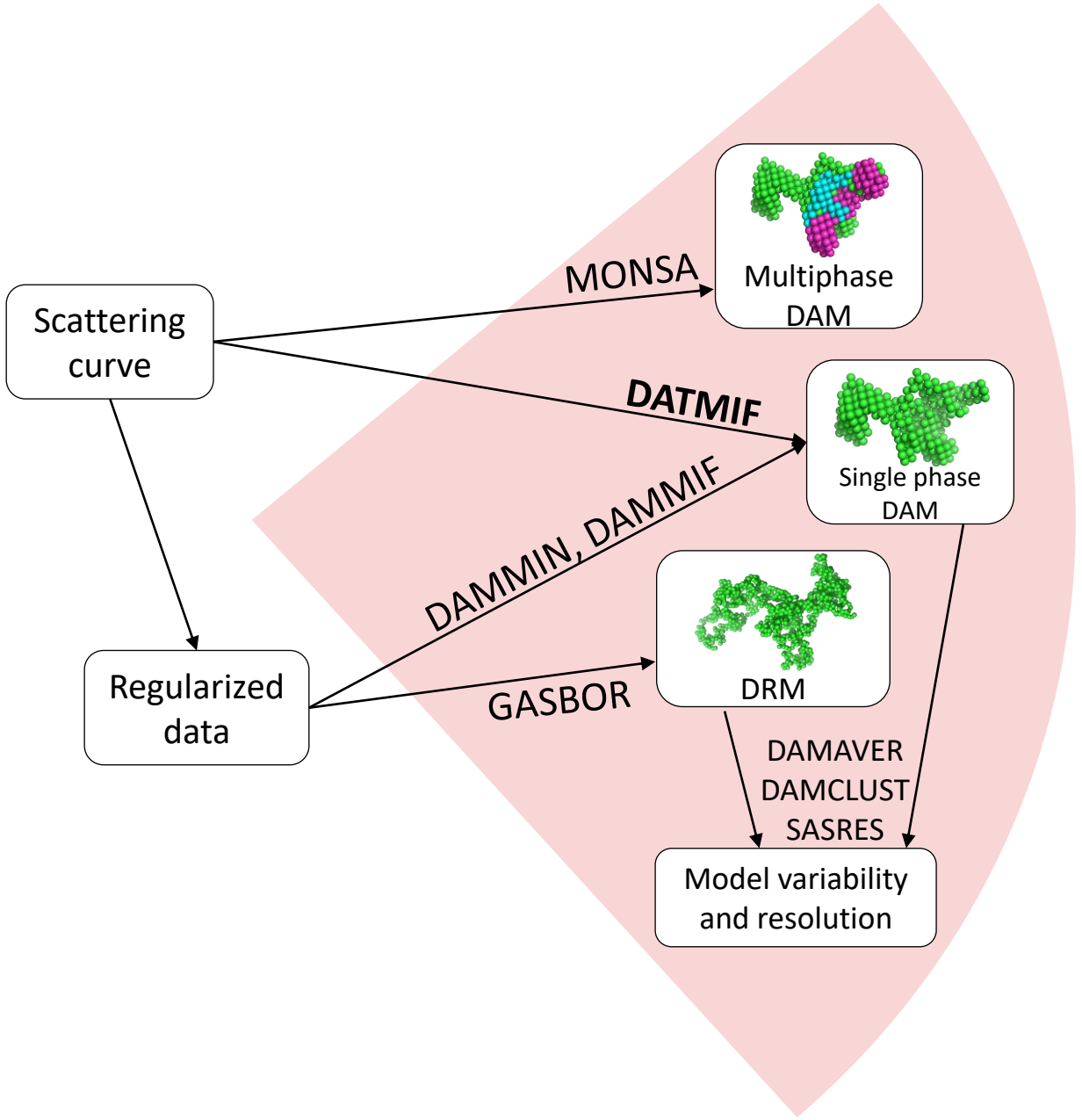
Ab initio modelling

DATMIF

- bead modelling using experimental data directly
- Can be used to cross-validate bead models from other methods

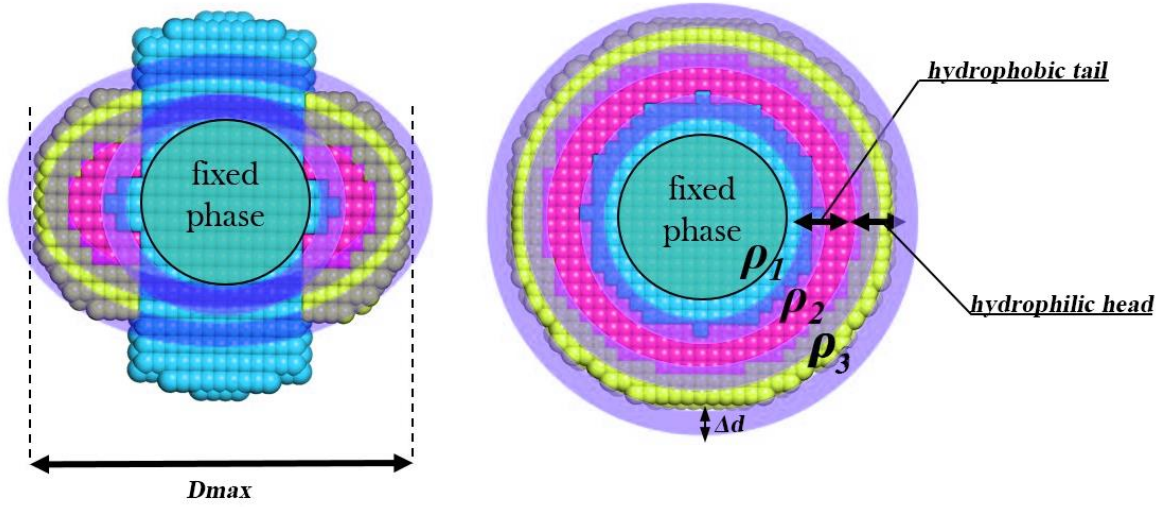
Usage

datmif --dmax=<Dmax> <SAS datfile>



Ab initio modelling

- Auxiliary tool: **DAMEMB**
  - Builds initial bead model of a membrane protein, for further refinement by MONSA
  - Thickness of the detergent phases may be specified



Hybrid modelling

SREFLEX

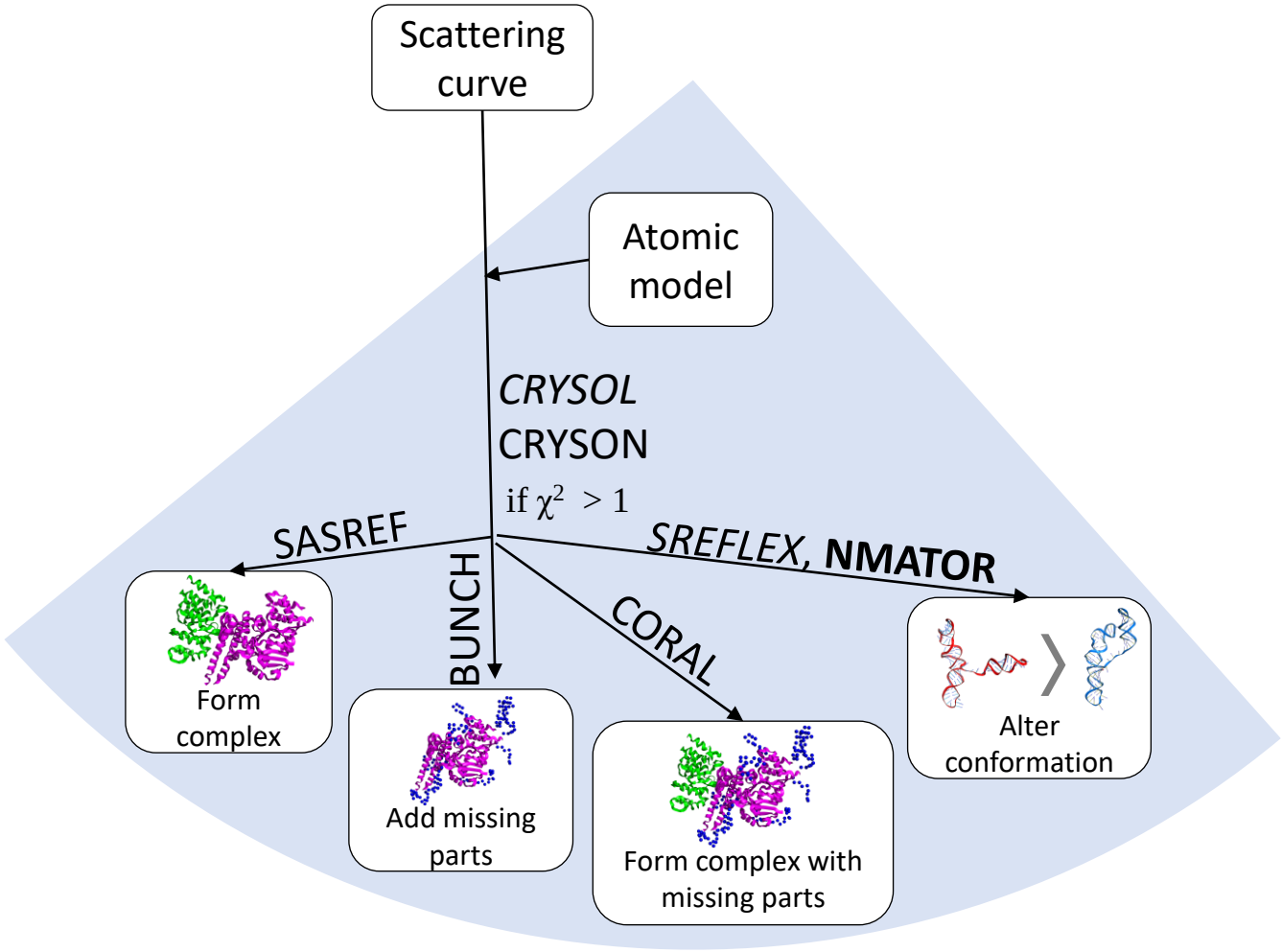
- Models conformational change as a set of coordinated movements in Cartesian space

Update: pool mode

- Can generate a pool of conformations for flexibility/mixtures analysis

Usage

sreflex -P <max # of conformers> <PDB file>



Hybrid modelling

NMATOR

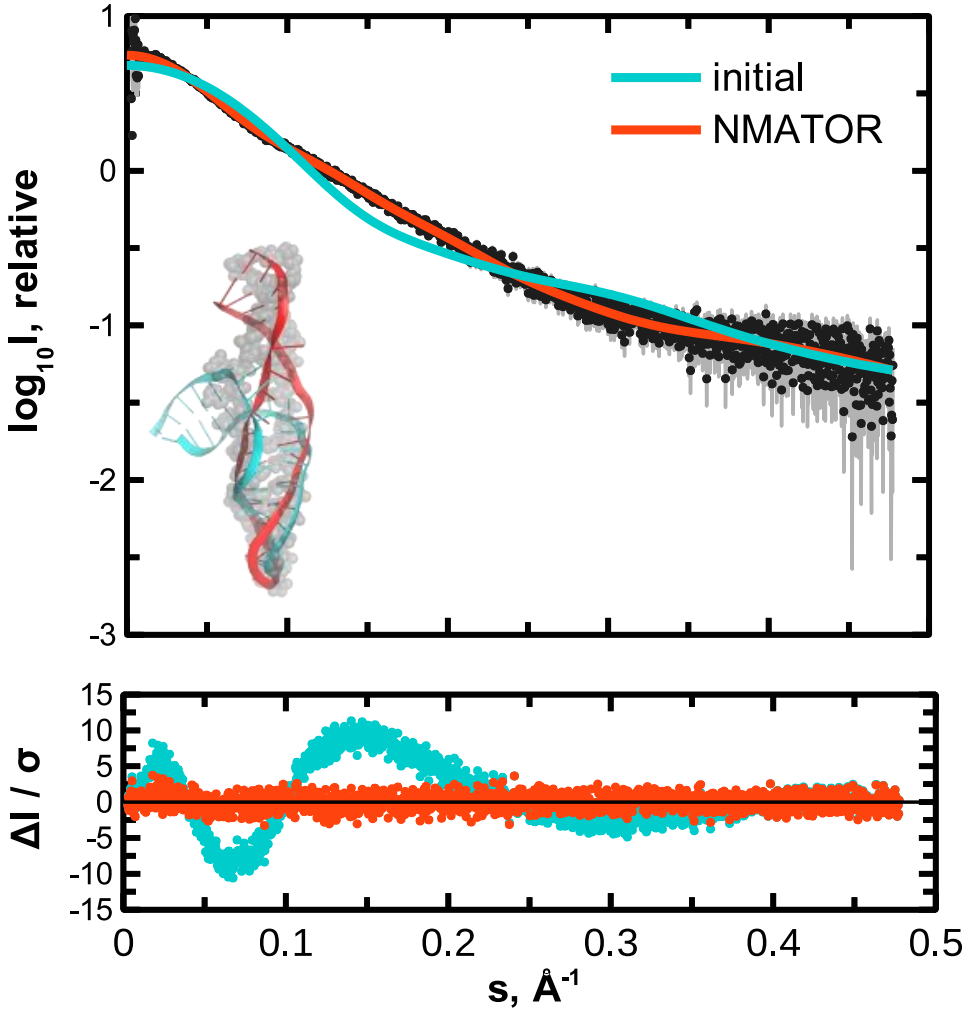
- **N**ormal **M**ode **A**nalysis in **TOR**sion angle space
- Models conformational change as a set of bulk dihedral angle rotations

Use cases

- single-strand RNA molecules, or cases that are too “broken” in SREFLEX

Usage

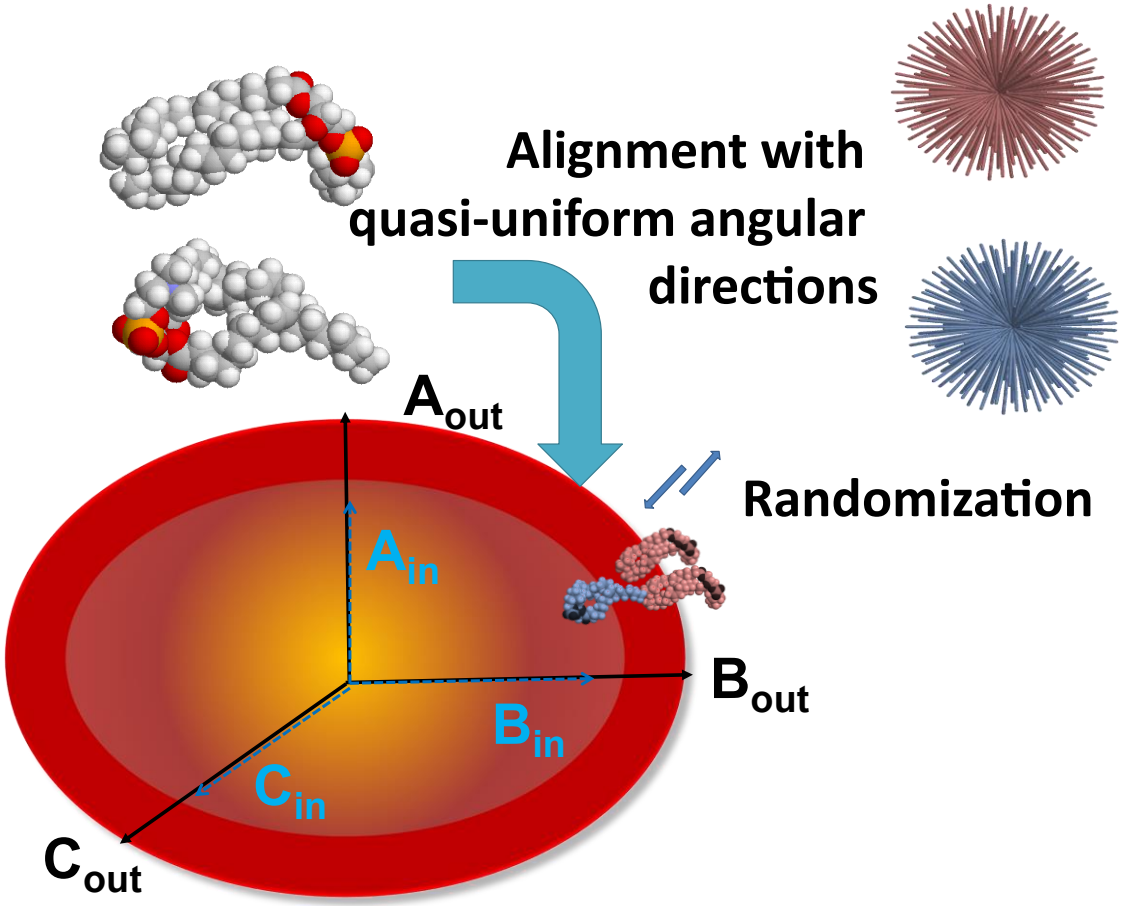
nmator <PDB/mmCIF file> fit <SAXS data file>



Hybrid modelling

Auxiliary tool: **ELLLIP**

- Builds ellipsoidal liposomes (or other bicellar systems) from atomic structure of building blocks

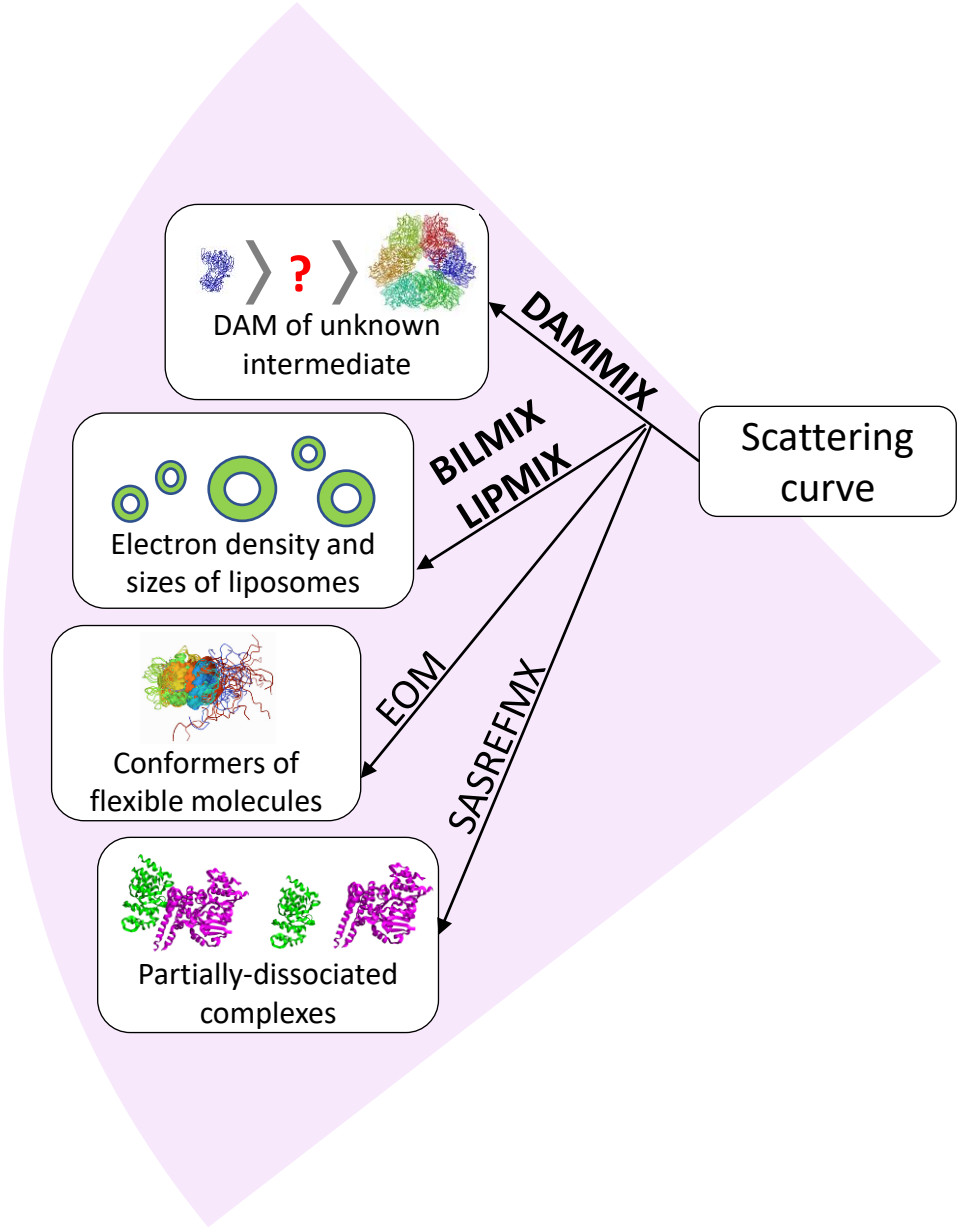


Petoukhov et al (2020) Crystallography Reports, 65, 258-263.

Mixtures analysis

New programs

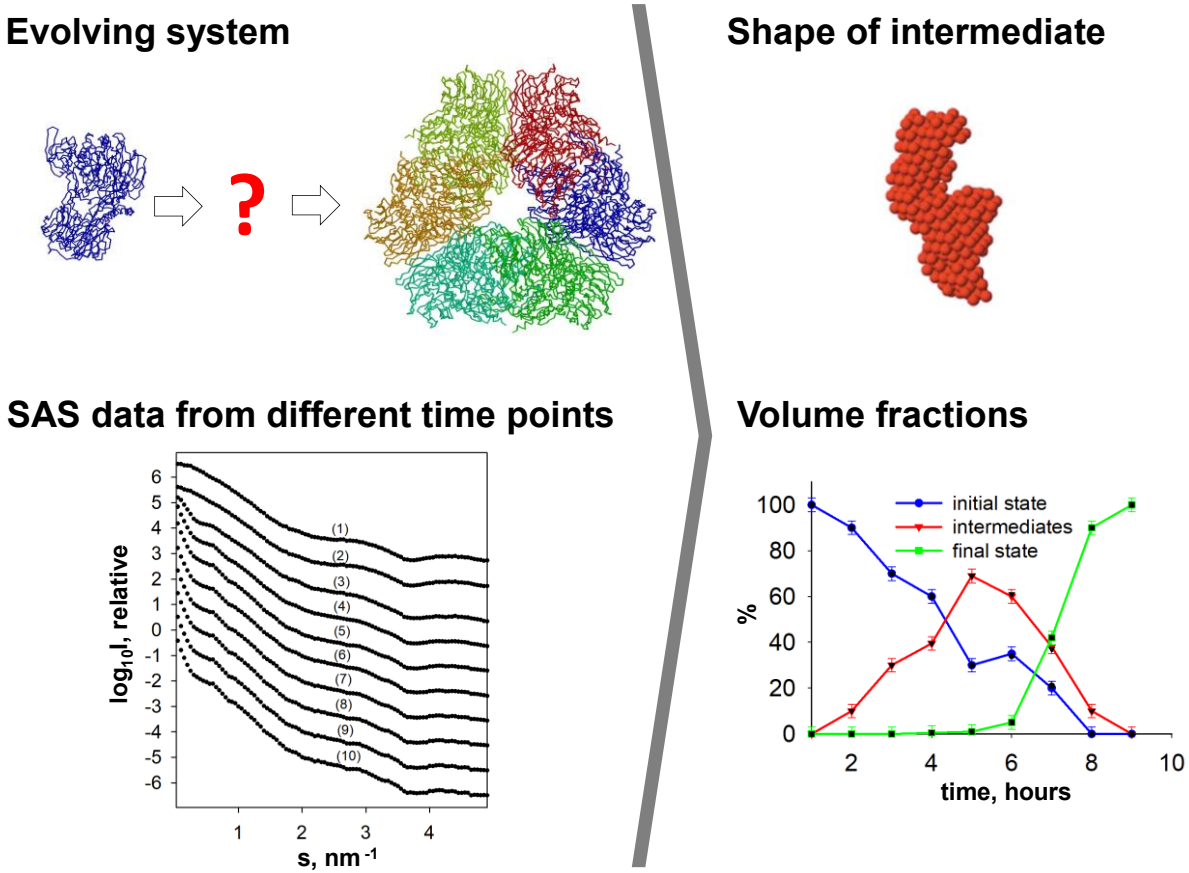
- DAMMIX
- BILMIX
- LIPMIX



Mixtures analysis

DAMMIX

- Builds *ab initio* model of an intermediate, given known endpoints and SAS time course data

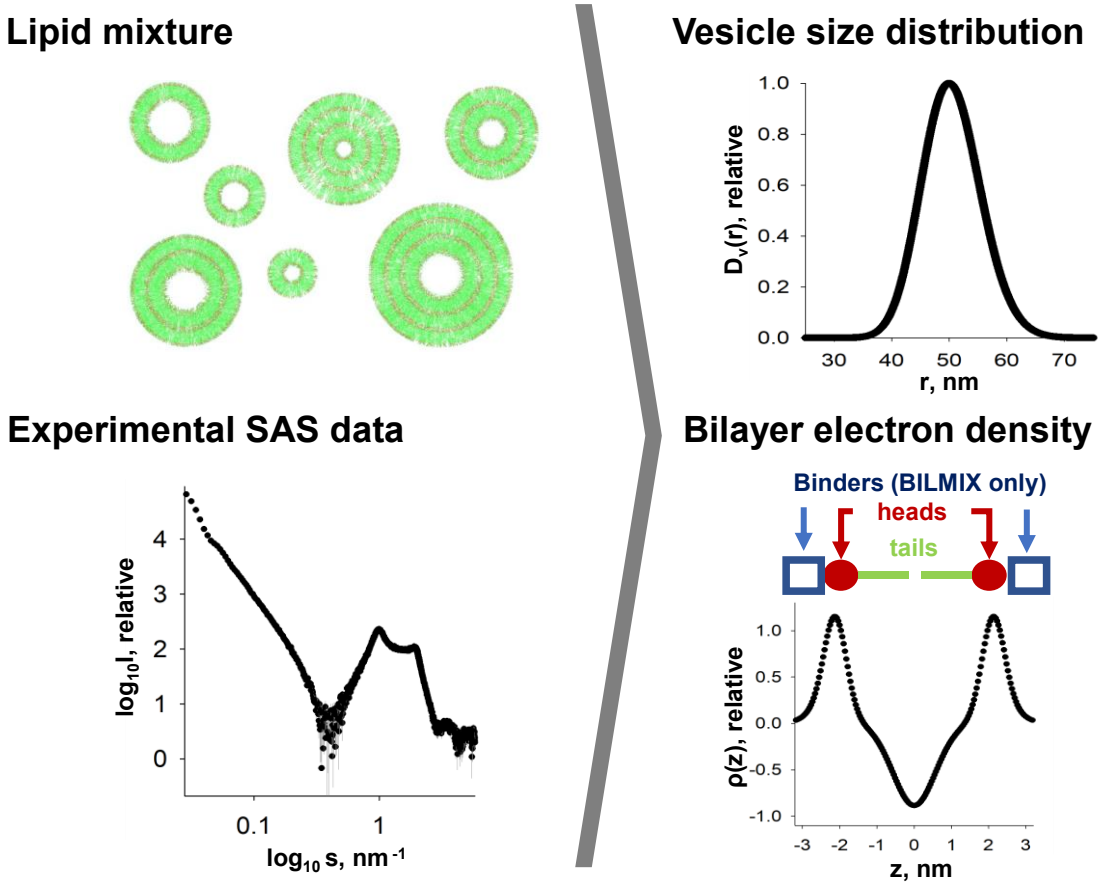


Konarev & Svergun (2018) IUCrJ, 5(4), 402-409

Mixtures analysis

LIPMIX and BILMIX

- model the size distribution ($D_v(r)$) and electron density profiles ($\rho(z)$) of liposomes
- BILMIX: for anisotropy
- LIPMIX: for multi-layered liposomes



Konarev et al (2020) JAC, 53(1)

mmCIF support

- Native read support: BUNCH, NMATOR
- CIF2PDB
  - Converts mmCIF files to PDB format to facilitate use by other ATSAS programs

Summary

New programs

- data simulation
- specialized modelling applications (nonproteins and/or mixtures)

Technical updates

- Improved GUI (Primus)
- Partial mmCIF support

Access:

- Download: https://www.embl-hamburg.de/biosaxs/software.html
- Run on cluster (ATSAS Online)
- Feedback welcome at SAXIER forum