refnx – The Next Generation of Reflectometry Analysis Software

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- Simultaneous co-refinement of Neutron and X-ray data
- Bayesian statistics for uncertainty quantification and model selection

Data Science Software

Python has exploded in popularity for data science. refnx leverages well tested and high performant libraries such as:

numpy + scipy → array computing and least squares

emcee, dynesty, pymc3 → Bayesian statistics

schwimmbad → MPI for parallelised cluster computing

refnx iis free, working on Linux/macOS/Windows.

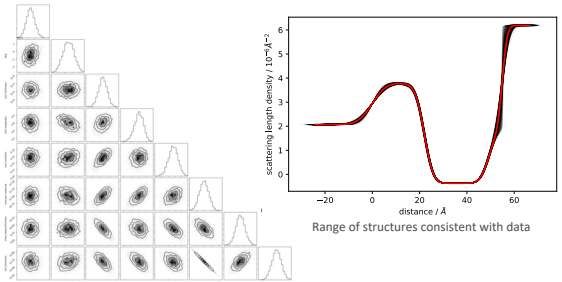
Bayesian statistics

$$p(\theta \mid D, I) = \frac{p(\theta \mid I)\, p(D \mid \theta, I)}{p(D \mid I)}, \quad p(D \mid \theta, I) = -\frac{1}{2}\sum_n \left[\left(\frac{y_n - y_{\mathrm{model},n}}{\sigma_n} \right)^2 + \log(2\pi\sigma_n^2) \right].$$

Encodes knowledge about system as a (prior) probability distribution (constraints).

Estimates the parameter (posterior) probability distribution using Markov Chain Monte Carlo.

Can compare different models and choose which is best.

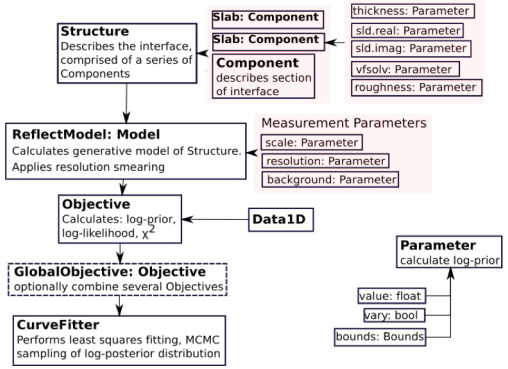


Corner plot showing probability distributions for parameters

Range of structures consistent with data

- Enables *REPRODUCIBLE RESEARCH*
- Open source, Python based with analyses performed in *Jupyter* notebooks, a Qt GUI, or scripts

Modular design



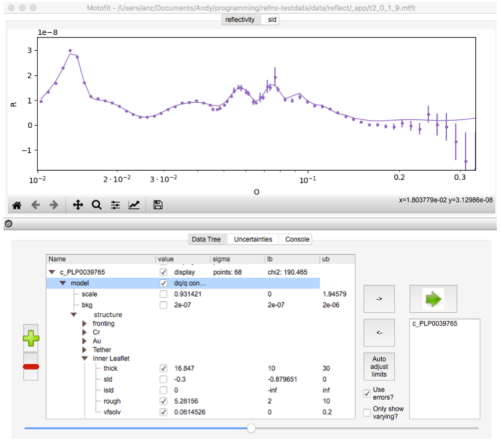
Structures are a series of *Components*, each of which describes a subset of the interface.

- **Slab** – uniform SLD over a set thickness.
- **Spline** – freeform description of SLD profile using splines.
- **LipidLeaflet** – describes a head/tail region of an amphiphile. Parameterised using Area Per Molecule to ensure 1:1 head to tail equivalency.
- **FreeformVFP** – volume fraction profile modelling of a polymer brush, adsorbed amount is bound by a Gaussian prior.

Different interfacial roughnesses are available:
Gaussian/Tanh/Linear/Exponential/Sinusoidal/Step

- Modular construction of structural models, problem specific parameterization (e.g. LipidLeaflet)
- Mixed area models

Qt GUI



- GUI offers easy setup for novice users, YouTube video tutorials
- Batch fitting/corefinement

Jupyter Notebooks

- Notebooks mix executable code, narrative text, and graphics within a single document.
- Distributing Notebooks as supplementary information facilitates reproducible research, readers can do the same analysis as you did.

https://github.com/refnx/refnx

Nelson, A. R. J. & Prescott, S. W., refnx: neutron and X-ray reflectometry analysis in Python, *Journal of Applied Crystallography*, **2019**, *52*, 193-200