Development of CORFUNC

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The Corfunc programme [1] is an application in the CCP13 suite designed to perform correlation function analysis on one-dimensional SAXS and SANS data in order to yield physical parameters of the specimen in terms of an ideal lamellar morphology. The correlation function calculated by the programme is essentially a Fourier transform of the input data. In order to achieve this overall aim, the task is split into three logical parts:

1. *Extrapolation*: prior to performing the transform, the data curve must be modelled to remove the restriction of finite q, and finite intensity values. The programs 'tailjoin' and 'tailfit' fulfil this role: with tailjoin being responsible for the shape of the curve as q tends to zero, and tailfit modelling the curve as it tends to infinity.

2. *Fourier transform*: the program 'transform' performs a Fourier transform on the extrapolated data, yielding the one-dimensional correlation function, Γ_1. (It can also re-transform the result back into a smoothed copy of the extrapolated data).

3. *Interpretation of Γ_1*: the program 'extract' interprets the features of Γ_1, based on an ideal lamellar morphology.

The Corfunc program has been written in modular form in order for individual elements of it to be edited without disrupting the application as a whole. (Indeed, many parts of it may be edited without necessitating a full re-compile, or even swapped-out at run-time for a module with an identical programmatic interface, but with a dissimilar purpose.)

As far as the end user is concerned the compartmentalisation of Corfunc is irrelevant. In order to remove the user from unnecessary exposure to the internal workings of the application, a Java GUI (Graphical User Interface) is provided. The programming language Java was chosen as this affords a compile once, run everywhere strategy (at least for the interface: the underlying command-line programs still require compilation for each end-user platform).

It is the modular nature of Corfunc we shall be exploiting in order to augment its functionality to encompass the study of adsorbed layers in colloidal dispersions. In this addition to Corfunc's scope we are primarily interested in harnessing its curve-fitting ability, if not, necessarily, developing its existing direction: we then only need to provide an alternative 'transform' module in order to expand the program's potential to incorporate new uses in the area of colloidal dispersions.
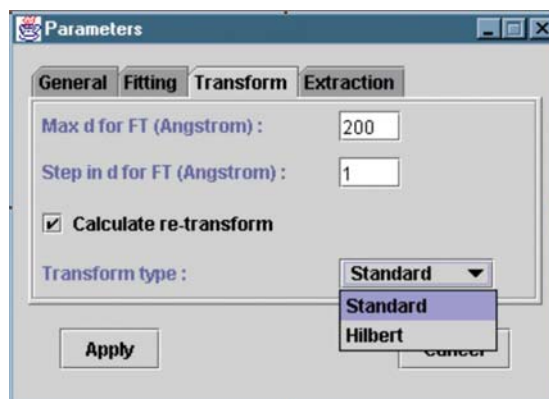

Figure 1. The edited transform parameters pane showing the new Hilbert option.

The particular area we are interested in concerns the manipulation of small-angle scattering data to yield information about the radial distribution of adsorbed layers of polymer or surfactant molecules. Using a Hilbert transform based on a method discussed in King, *et al.*, [2] we can directly substitute the existing transform module and then plot the results via Corfunc's in-built display procedures, without having to edit the way Corfunc deals with transform output files.

An important caveat to bear in mind with this new development is that existing users may be unsure how to respond with the new 'Hilbert' option that appears in the interface. In order to lessen the risk that an injudicious selection of transform may cause, Corfunc's online help files have been edited to include a description of the purpose and relevance of the new functionality.

References

[1] T. M. W. Nye, *SAXS Correlation Function Analysis: Notes on the Software at Daresbury*.
http://www.ccp13.ac.uk/software/program/corfunc.html

[2] S. M. King, P.C. Griffiths, and T. Cosgrove. Using SANS to study adsorbed layers in colloidal dispersions, in "*Applications of Neutron Scattering to Soft Condensed Matter*", ed. B.J. Gabrys, Gordon & Breach Science Publishers, Amsterdam, 2000.