TITLE and type of activity (Networking, Joint Research development): Multi-purpose software for global and complementary structural data analysis

Leading beneficiary: ILL

Partners: TO BE CONTACTED : ESS –– ISIS – Univ. Politech. Marche – TUB (Gradzielski group) – Lund Univ. (Schurtenberger) - ESRF

Estimated budget (in person months, other direct cost) and tentative distribution per partner ! 2 PostDocs? *Ask Mark if feasible for students....*

Abstract of your innovative activity:

More and more scientists from diverse scientific areas in soft matter science are attracted by scattering techniques available at large scale facilities (LSF) to investigate the intimate structure of matter. Many of them are biologists, chemists, pharmacologists that often do not have skills in programming and writing their own code to analyze data collected at LSFs.

Data analysis is nowadays performed by using several software applications, mostly developed by instrument scientists and poorly integrated among different instruments. This way of development results in software applications difficult to be used by non-expert researchers in programming and suffers of many limitations (reliability of error parameters, stability, accuracy and so on).

We must go beyond the current lack of performances and standardization bearing in mind that nowadays research is devoted to complementarity. In terms of structural investigation of soft matter systems the joint use of neutrons, visible lights and X-rays is essential to investigate complex systems. In turns it would be extremely useful to have a unique tool to analyse simultaneously all the datasets originated by the same samples probed with complementary techniques. Such a software application does not exist at the present day, neither on the market nor as free tool.

Different facilities and university researchers with excellent skills in scientific data analysis programming will be involved in this project. At the beginning the development will be focused on the joint and simultaneous analysis of small angle neutron scattering, small angle X-ray scattering and static light scattering. The same software will be used to analyse reflectivity data collected by using neutrons, X-rays and visible light. The software will fill the gap present between different data analysis method and will provide an easy and user friendly environment open to all researchers. This will in turn result into a more efficient data analysis strategy, boosting the research activity of all the community involved and will also have a positive impact on the data standardization process already started among the European LSFs.