

SFF analysis of a small angle scattering data from phospholipid vesicles systems: online interface and parallel implementation

Friday 15 October 2021 10:45 (15 minutes)

The study of phospholipid vesicles is one of the hot topics of modern nano- and biophysics in connection with the numerous applications of these objects in medicine, pharmacology, and cosmetology. One of the most effective and intensively used methods in the last decade for studying the structure and properties of vesicles from small-angle neutron scattering (SANS) data is the separated form factor (SFF) method.

The Windows-based online interface for convenient work with a respective Fortran program is presented, which implements the fitting of the structural parameters of polydisperse vesicular systems according to experimental SANS data within the SFF model based on the standard local minimization program DFUMIL from the JINRLIB electronic library.

Due to the fact that, with a large amount of experimental data, the analysis of SANS spectra can take a significant amount of time, a parallel implementation of the adjustment of the RFF parameters based on the MPI parallel programming technology has also been developed.

The prospects of creating an information system based on the HybriLIT platform (LIT, JINR, Dubna) are discussed, which implements efficient parallel processing of small-angle spectra with a convenient web interface for entering input parameters and visualizing the results.

Primary author: BASHASHIN, Maxim (JINR)

Presenter: BASHASHIN, Maxim (JINR)

Session Classification: Mathematical Modeling and Computational Physics

Track Classification: Mathematical Modeling and Computational Physics