



Contribution ID: 465

Type: **Poster**

## Updates in SASfit for fitting analytical expressions and numerical models to small angle scattering patterns

*Tuesday 21 March 2023 16:00 (2 hours)*

Small-angle scattering is an increasingly common method for characterizing particle ensembles in a wide variety of sample types and for diverse areas of application. SASfit has been one of the most comprehensive and flexible curve fitting programs for decades, with many specialized tools for various fields. Here, a selection of enhancements and additions to the SASfit program are presented that may be of great benefit to interested and advanced users alike: (a) further development of the technical basis of the program, such as new numerical algorithms currently in use, a continuous integration practice for automated building and packaging of the software, and upgrades on the plug-in system for easier adoption by third-party developers; (b) a selection of new form factors for anisotropic scattering patterns and updates to existing form factors to account for multiple scattering effects; (c) a new type of a very flexible distribution called metalog, and regularization techniques such as the expectation-maximization method, which is compared with fits of analytical size distributions via the non-linear least-squares method; and (d) new structure factors, especially for ordered nano- and meso-scaled material systems, as well as the Ornstein–Zernike solver for numerical determination of particle interactions and the resulting structure factor when no analytical solution is available, with the aim of incorporating its effects into the small-angle scattering intensity model used for fitting with SASfit.

**Author:** Dr KOHLBRECHER, Joachim (Laboratory for Neutron Scattering and Imaging)

**Co-author:** Dr BRESSLER, Ingo (BAM Berlin)

**Presenter:** Dr KOHLBRECHER, Joachim (Laboratory for Neutron Scattering and Imaging)

**Session Classification:** Poster session TUESDAY

**Track Classification:** Neutron Instrumentation, Optics, Sample Environment, Detectors, and Software