The MLZ Scientific Computing Group: Software for GISAS, and Further Projects

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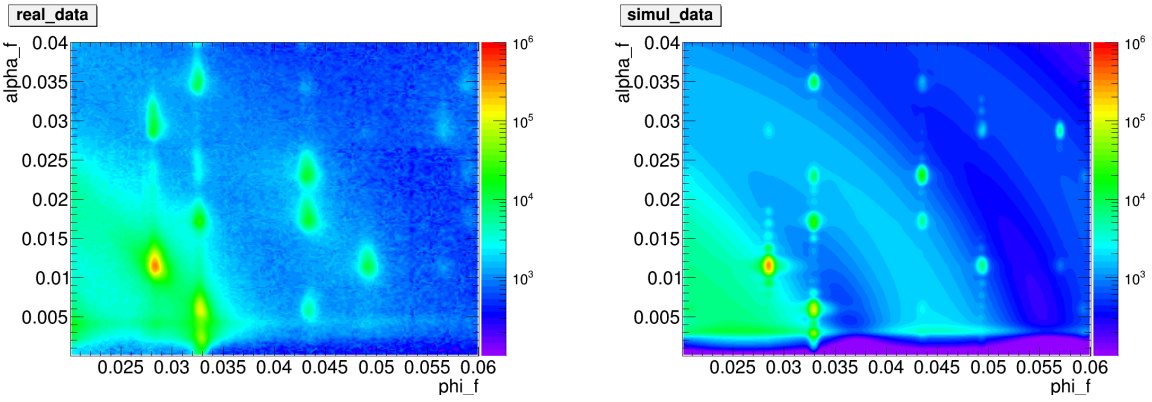
Since February 2013, the collaboration of German research institutions for the scientific use of the neutron source FRM II has a new name: Heinz Maier-Leibnitz Zentrum (MLZ). As part of this collaboration, Forschungszentrum Jülich has created a new Scientific Computing Group that will support all scattering instruments of the MLZ.

The first big project of our group is the development of a new software for simulating and fitting grazing-incidence small-angle scattering (GISAS). This project is embedded in workpackage 3 of the High Data Rate Processing and Analysis Initiative (HDRI) of the Helmholtz-Gemeinschaft, and the final product will serve synchrotron (GISAXS) as well as neutron (GISANS) instruments.

The name of the software, BornAgain, indicates the central rôle of the distorted-wave Born approximation (DWBA) in the physical description of the scattering process. The software provides a generic frame for modelling multilayer samples with smooth or rough interfaces and with various types of embedded nanoparticles. In this way, it reproduces and enhances the functionality of the present reference software, IsGisaxs by Rémi Lazzari, and lays a solid base for future extensions in response to specific user needs. The first public release will be presented in April 2013 at workshop on GISAS data analysis organized by the SC group. The next development step, planned for 2013/14, will address polarized GISANS for the investigation of magnetic domains.



Grazing-incidence small-angle X-ray scattering from a mesocrystalline system (left, courtesy Elisabeth Josten et al.), compared to a BornAgain simulation (right). The mesocrystals have cylindrical shape and a size of about 1000 nm; they are vertically oriented, and randomly distributed on a silicon substrate. Each of these mesocrystals consists of an FCC lattice composed of 5 nm spherical particles.

In the second part of my talk, I will outline ideas for our next projects, in particular for data reduction and analysis in inelastic scattering (mainly time-of-flight and backscattering experiments).

Finally, I will mention our contributions to more generic open-source software, like the library libkww for the efficient and precise computation of the Laplace-Fourier transform of the stretched exponential function.