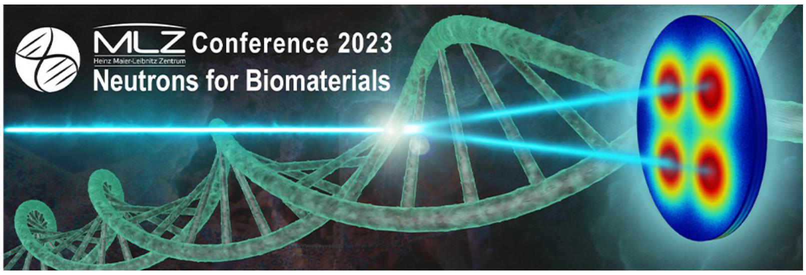

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Probabilistic classification of 2D Small-Angle Scattering Patterns

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X-ray and neutron scattering are widely used powerful techniques for probing the physical structure of materials at the molecular and supramolecular scale. With the simultaneous advent of high-speed detectors, previously unimaginable time-resolved in situ and high throughput photon and neutron experiments have become possible, with the subsequent explosion of data volumes. Data analysis is becoming the most serious bottleneck on the way from experiment to scientific insight and final publication. We aim to provide rapid machine learning-based data classification to (i) guide decisions during the course of an experiment and to (ii) guide users as to which models are most appropriate for subsequent data analysis.

The main challenge of AI-assisted data analysis is that simulated and experimental data come from different distributions. Thus, in general case, model trained on simulated data will highly probably have a poor performance on the experimental data. We developed a methodology where the small-angle scattering patterns or 2D detector data are first transformed from (qx,qy) into (r,phi)-coordinates to become independent of the specific beam position on the detector and the specific detector pixel array format. The subsequent Fourier transform transforms the data from (r,phi)- to a real-space representation in Carthesian (x,y) coordinates. This makes use of Friedel's law and the Fourier shift theorem for a reduced presentation of the data. It is thus possible to operate with one training set for different instruments and different detectors. We used a broad range of experimental and simulated 2D-scattering data for spheres, ellipsoids, isotropic and oriented cylinders, as well as ordered lattice structures consisting of spheres, cylinders or lamellae of different degree of positional and orientational order and polydispersity.

In the present work we compare performance of probabilistic classification using variational inference neural networks for different data representations. We show, that the transformed data can be better classified compared to the original 2D-detector data, enabling a reliable fast classification of scattering patterns with the possibility for a subsequent automatized data analysis with the selected models.

Author: GANEVA, Marina (JCNS at MLZ, Forschungszentrum Jülich GmbH)

Co-authors: WAGENER, Michael (Forschungszentrum Jülich); FÖRSTER, Stephan (Forschungszentrum Jülich)

Presenter: GANEVA, Marina (JCNS at MLZ, Forschungszentrum Jülich GmbH)

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