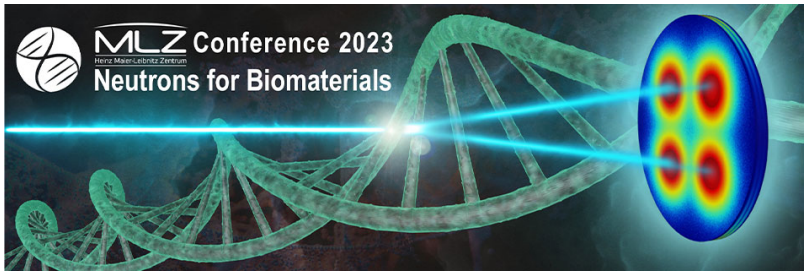

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Optimization of SANS data in multiparameter spaces by Monte Carlo and Bayesian modelling

Small angle neutron scattering (SANS) is a powerful experimental technique for the investigation of soft matter and in particular biomaterials thanks to the high contrast between hydrogenated and deuterated components and its spatial resolving power in the nm scale (1-100 nm). We have used SANS to obtain details on the morphology of biomaterial nanostructures which often form multiple populations of particles in size and shape and furthermore can be organized hierarchically [1-3]. Model-dependent scattering functions which cover a vast number of scattering objects, e.g., spheres, cylinders, core-shell micelles, fractal structures etc. and their combinations are used to fit the collected experimental data, to confirm the existence of the different structural species and probe the organization at different length-scales. Monte Carlo simulated annealing algorithms have been proven a versatile tool for SANS data optimization, however, increasing the complexity of the scattering models leads to an increase of the number of the optimization parameters. This brings up the question of the independence between the fitted parameters and the validity of the applied models. In order to clarify such issues in data analysis, a Markov Chain Monte Carlo (MCMC) algorithm [4, 5] is applied to obtain the posterior distributions of the fitted parameters and naturally extract their uncertainties and mutual dependencies. The application of Bayesian inference will be presented with examples from vesicular systems with polydisperse size and lamellarity [6, 7] and self-assembling doubly responsive copolymers [8]. These works illustrate the potential of Bayesian analysis for the optimization of SANS from biomaterials using models with large number of optimization parameters.

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