Contribution ID: **24** Type: **not specified**

Survival of the FITtest: Can Evolution Teach Us to Fit SAS Data?

Wednesday, 17 December 2025 14:20 (20 minutes)

Small-angle scattering (SAS) curve fitting is frequently posed as a rugged, high-dimensional optimisation problem. In many practical cases, closely similar I(q) profiles can be produced by markedly different parameter combinations, highlighting the challenge of parameter degeneracies. Satisfactory solutions are rarely achieved without imposing constraints or introducing prior assumptions about the sample, acknowledging the complexity researchers face.

Genetic algorithms (GAs) have long been used in SAS data analysis. Indeed, GA usage can drastically simplify the analysis of experiments. However, standard single-population implementations (often bit-encoded) perform poorly as dimensionality and complexity increase or when the forward model involves strongly coupled continuous parameters. Here, it will be shown how strategies inspired by Darwinian Evolution (variation, selective pressure, adaptive mutation, spatial separation, and limited exchange) can be translated into computational optimisation schemes for SAS data. In particular, an island-model evolutionary algorithm is presented, in which multiple populations are evolved in parallel under distinct evolutionary pressures and represent different real-space modelling hypotheses. The Galápagos finches, a well-known example of adaptive radiation, inspire such a GA design. These design principles are then consolidated in STORM (Small-Angle Scattering Toolkit for Optimisation and Real-space Modelling), which implements a low-prior, user-friendly, evolution-inspired philosophy designed to provide robust SAS fitting in highly dimensional settings.

Abstract Title

Primary author: SANCHES PIRES, Rodrigo (European Synchotron Radiation Facility, ID02 beamline)

Presenter: SANCHES PIRES, Rodrigo (European Synchotron Radiation Facility, ID02 beamline)

Session Classification: Talks