



IDS for Neutron Reflectometry (ESTIA)

DMSC STAP — 2023/04/26

Andrew McCluskey ✉

Instrument Data Scientist - Reflectometry

@ andrew.mccluskey@ess.eu

♂ (he/him)



Current responsibilities

- Instrument Data Scientist for ESTIA 
- Project owner/lead developer EasyReflectometry 
- Lead organiser of DMSC Summer School 
- Independent research 

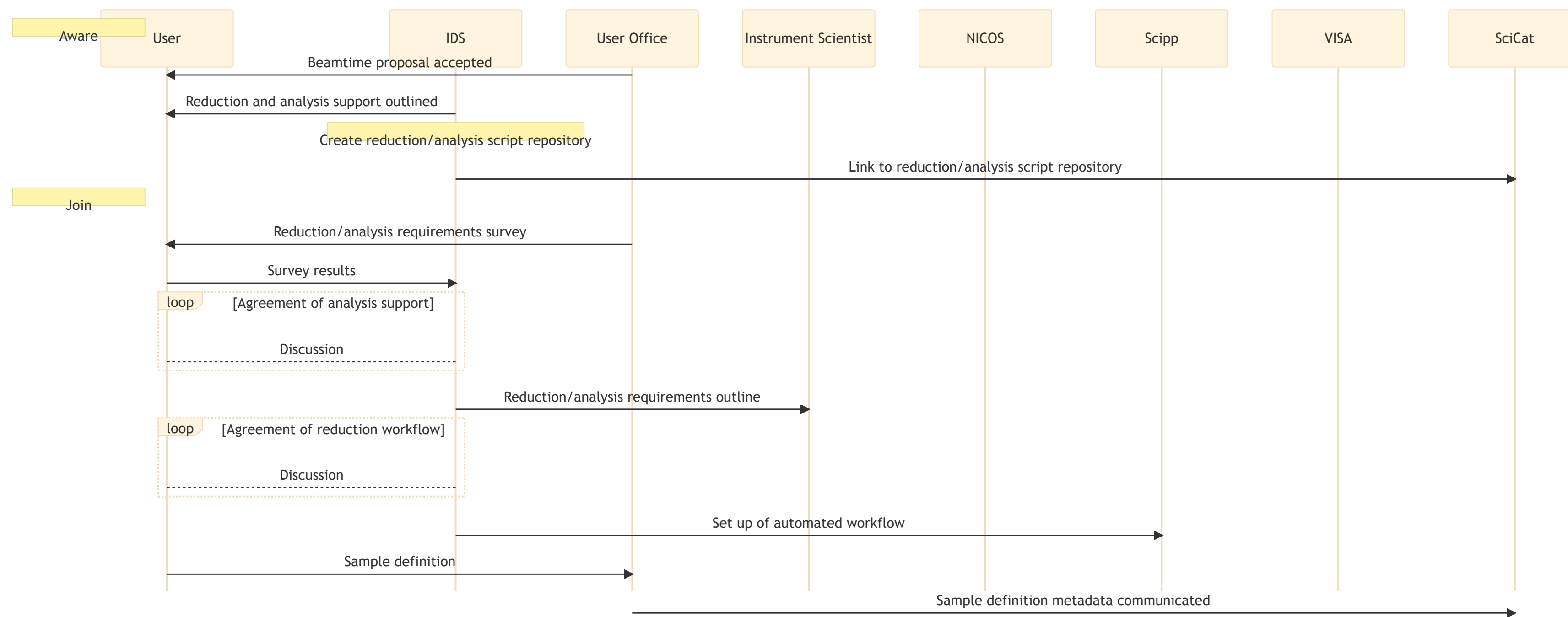


ESTIA Readiness



Service Blueprint

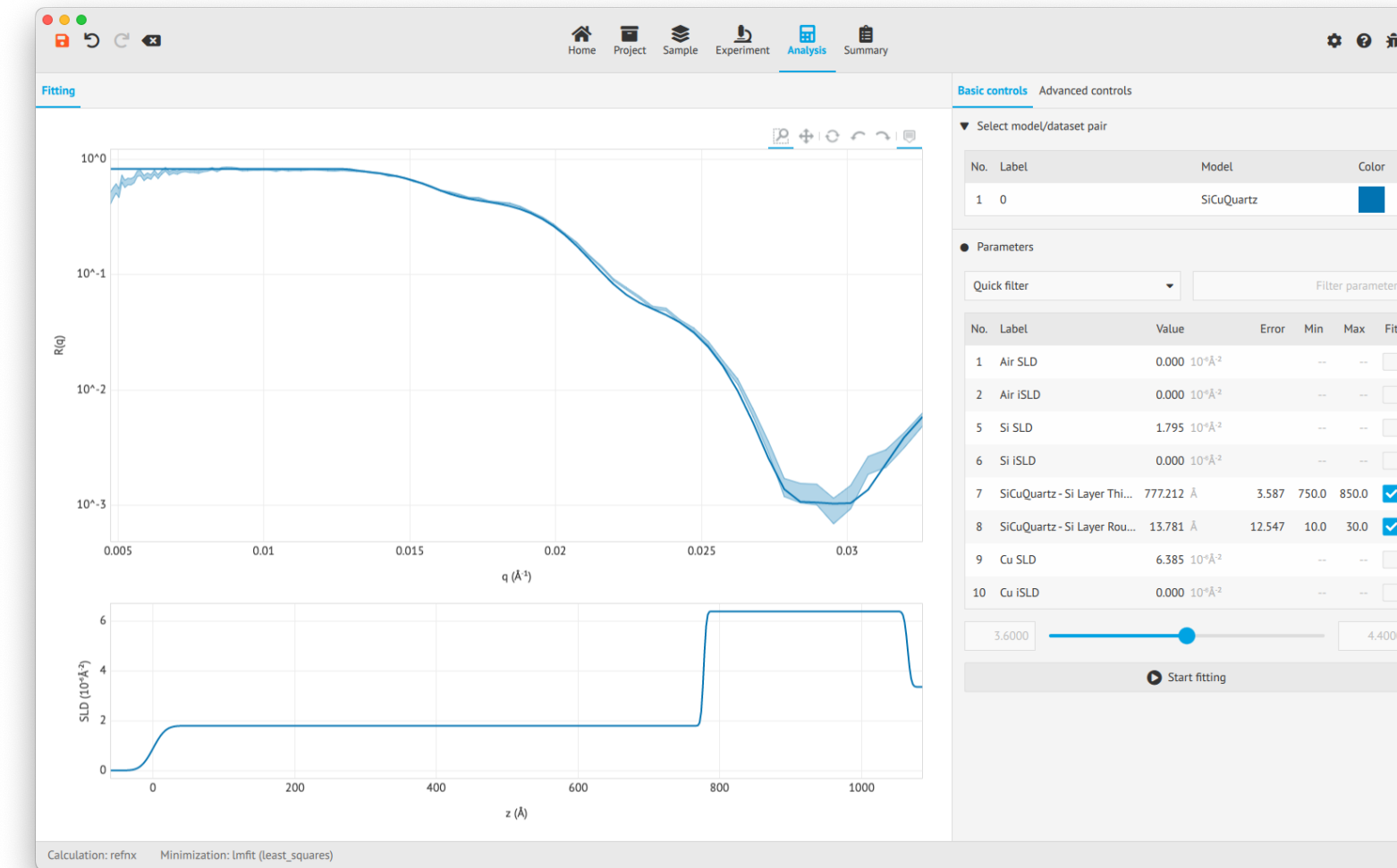
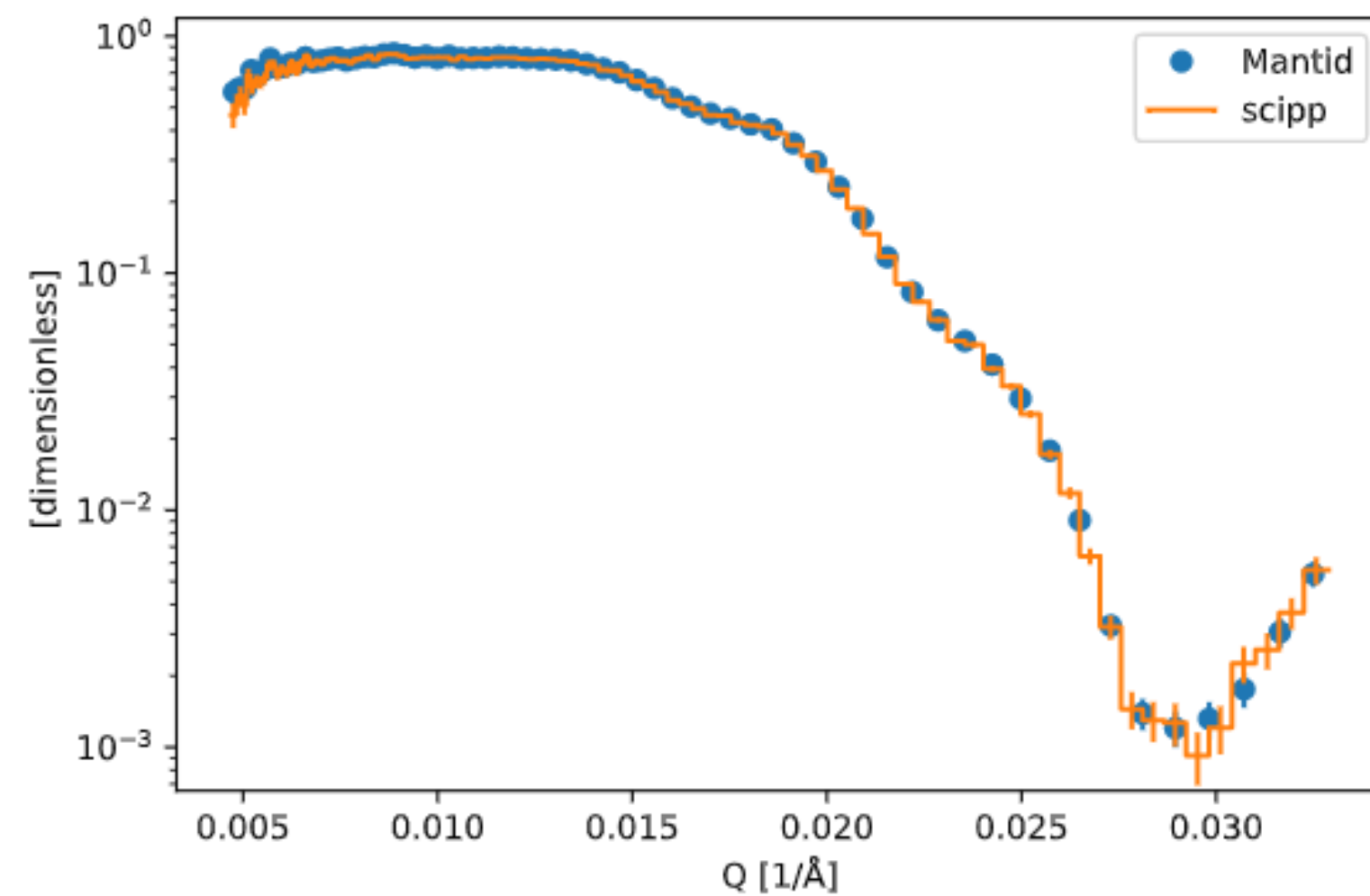
- Planning the interactions between the user and the data pipeline at ESS
- Four users types defined:
 - New users
 - Users with *complex* reduction/analysis requirements
 - Experienced users
 - Users looking to co-refine specular/off-specular/GISANS data
- **Next 6 months:** Finalise service blueprints, following STAP feedback





Data Reduction Workflows

- Eight potential operation modes for ESTIA
- Three binary options that should be considered in reduction:
Focusing mode / Polarisation / Pulse skipping
- Currently workflows exist for the 100 and 000 modes
- **Next 6 months:** Developing McStas simulations to cover the remaining modes



Data from OFFSPEC instrument, reduced with Mantid and `scipp`, the `scipp` reduced data was then analysed with EasyReflectometry.



Selene Guide Commissioning

- Integration of metrology cart and screwdriver robot for ESTIA Selene guide
- **Next 6 months:** Complete integration and start on guide optimisation software



A demonstration of the screwdriver robot in action.

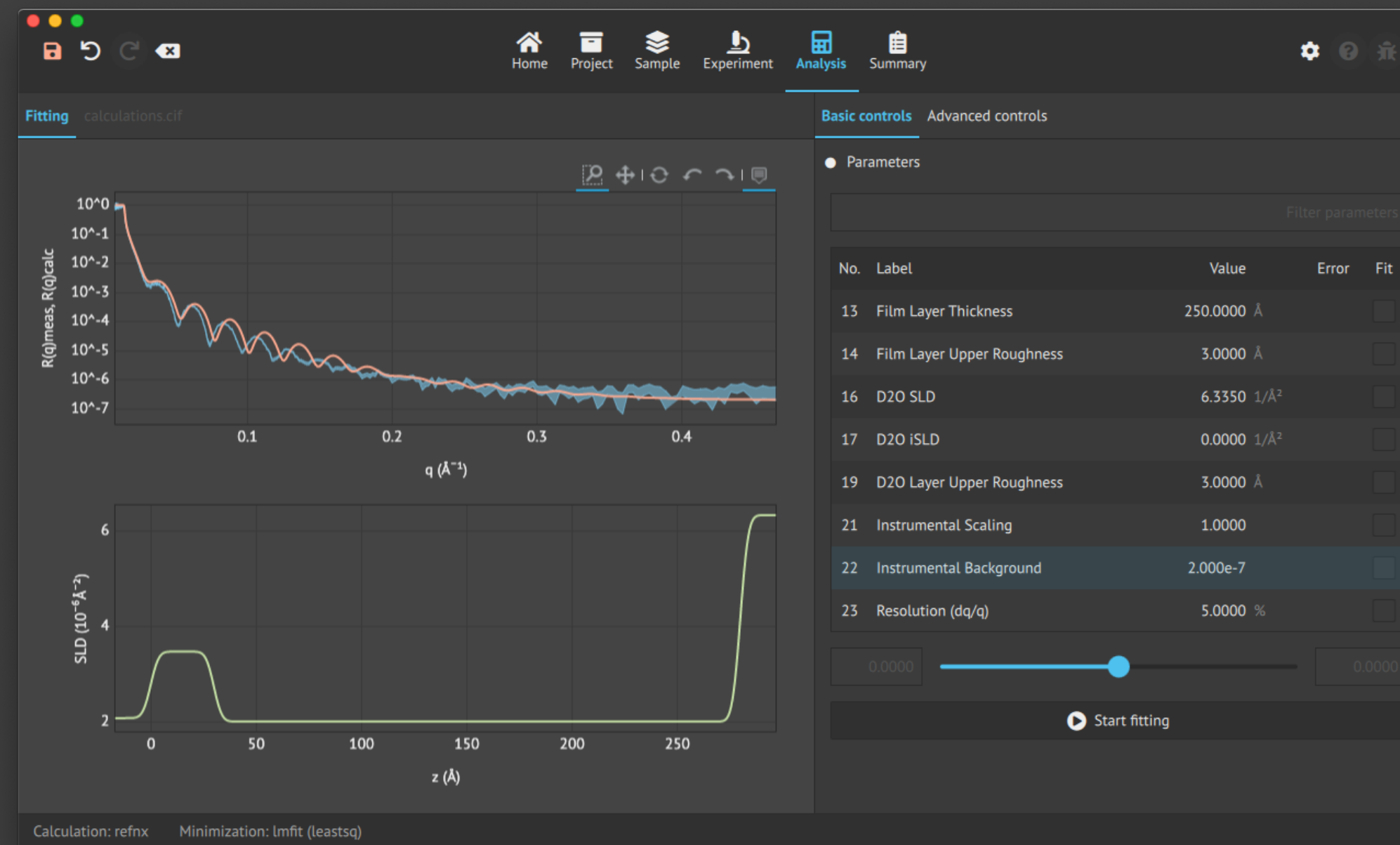


EasyReflectometry



EasyReflectometry

- Easy to use and extensible analysis package for reflectometry
- Built on successes of EasyScience/EasyDiffraction
- Functionality includes co-refinement, such as for multiple isotopic contrasts



The sample tab for the EasyReflectometry GUI interface.



Roadmap

- Outlines planned *functionality* for EasyReflectometry between now and SOUP
- **Next 6 months:** User experience enhancements and *real* user engagement
- **Next 12 months:** Development of magnetism support and Bayesian analysis



DMSC Summer School



Your data: from proposal to publication

- First week in September; space for 12 students (application covered)
- Funding from DanScatt and (possibly) Novo Nordisk and Carlsberg
- Underwritten by ESS/DMSC

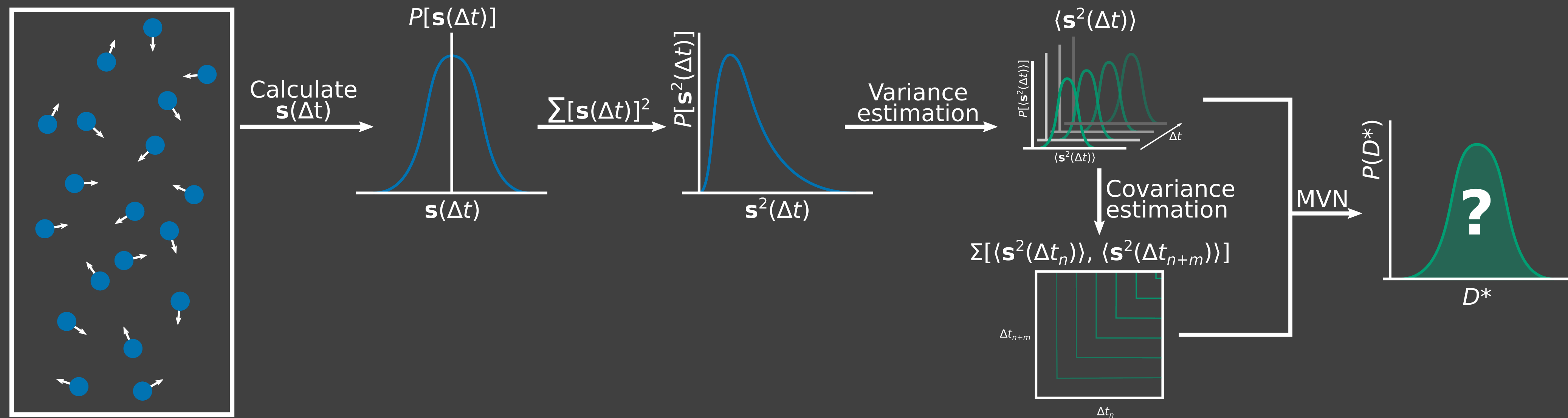


Independent Research



Physics-informed Machine Learning

- Linking atomistic data (simulations/etc) with neutron scattering
- Building on success in quantifying diffusion from mean-squared displacement
- **Next 6 months:** Applying for funding with collaborators from DTU and Queen Mary University of London





Five+ year plan

- 50 % joint position between ESTIA IDS and lectureship in local University
- Continue as EasyReflectometry product owner but with dedicated software developer
- Research- and teaching-active, while supporting users at ESTIA
- Complete an Ironman Triathlon 🏊🚴🏃



Contributors

Massimiliano Novelli

Jan-Lukas Wynen

Artur Glavic (PSI)

Fredrik Bolmsten

Simon Ward

Ben Morgan (Bath)

Simon Heybrock

Jos Cooper (ISIS)

Federico Rojas

Carina Lobley

Piotr Rozyczko

Sam Coles (Bath)

Keith Butler (QMUL)

Neil Vaytet

Jonas Petersson

Petra Aulin

Thomas Holm Rod

Andrew Sazonov

Ivano Castelli (DTU)

