Data processing for BEER

Updates since Sept 2025

Céline Durniak

IDS for DREAM and BEER

2026-04-21

Agenda

1 Status

2 Instrument simulation

3 ECDC tools

4 Data catalogue - Scicat

5 Data reduction - Scipp

6 Data analysis by Premek

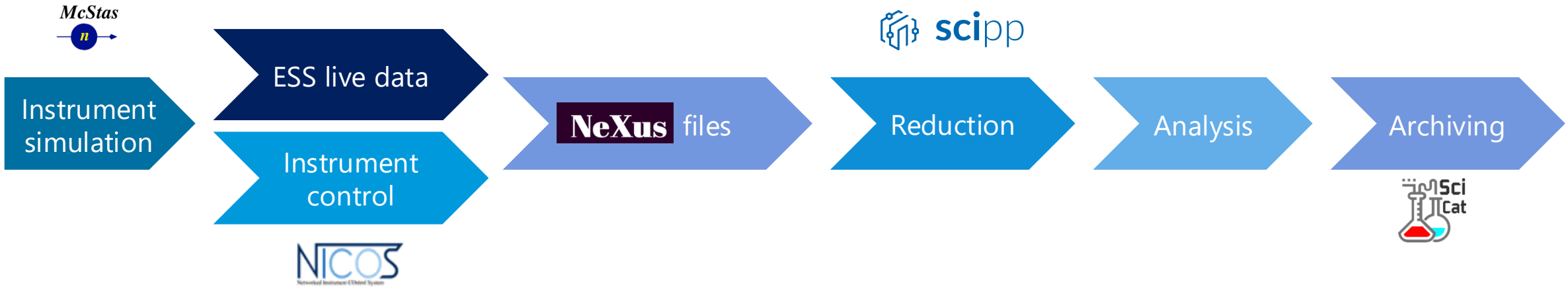
Acknowledgements

Contributors

- BEER instrument team
- McStas developers
- scipp developers
- Experiment Control and Data Collection (ECDC) team
- Scientific Information Management Systems (SIMS) team

Status - DMSC tools for BEER

Updates since last STAP (Sept 2025)



Status - DMSC tools for BEER

Updates since last STAP (Sept 2025)

- 3D detectors
- Day 1 configuration
- SE

Issue
- textured sample

Instrument simulation

No implementation for BEER

ESS live data

Instrument control

NICOS for BEER

- Day 1
- Specific SEs (hexapod)

NeXus files

Reduction

- Main software on VISA
- Instrument parameter files

Analysis

Archiving

Science cases
- Powder diffraction Q2/26
- Strain scan Q4/26
- Texture Q3/27
- In-situ /operando Q4/27

General features
Standard reduced format (stress/strain)

Training session for instrument team

- Experimental files
- Simulated files
- Reduced files
- Metadata

Legend

Done
Work in progress
To do

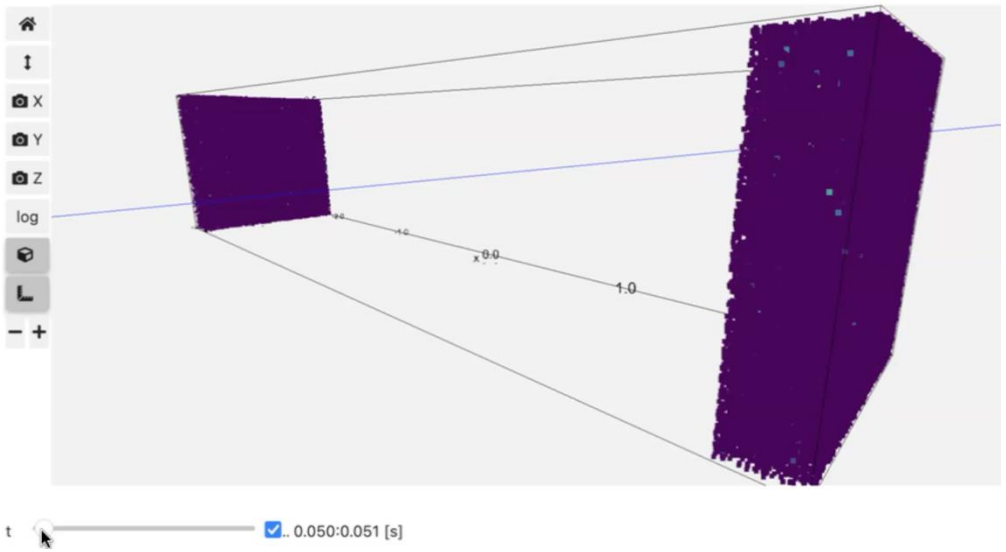
Instrument simulation

McStas

3D detectors

2 possible resolutions for each 2D panel

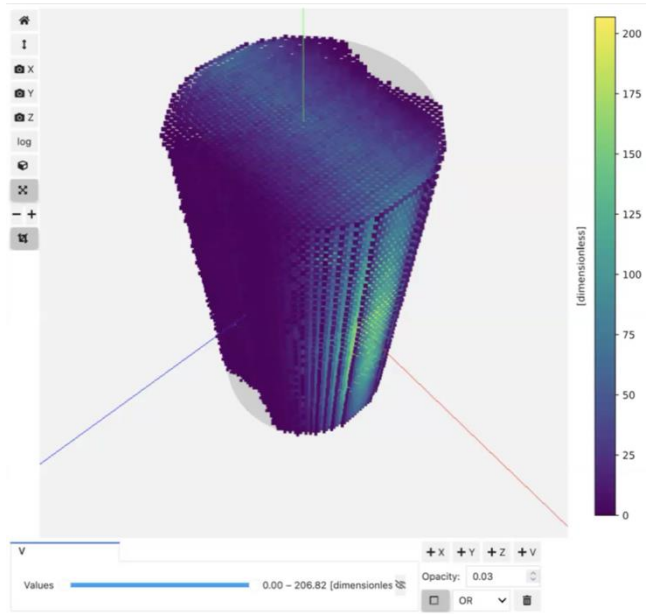
(3D view with Plopp / Scipp)



Gauge volume

x, y, z coordinates in the sample

(3D view with Plopp / Scipp)



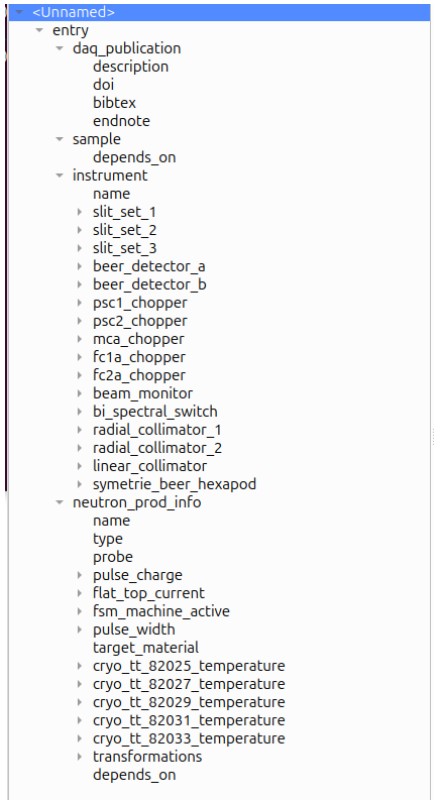
ECDC tools

CODA / NeXus files / NICOS (WIP)

- BEER in CODA (Continuous Data)

pipeline to test ECDC software (Event Formation Unit ➜ file writing through Kafka)

- Event Formation Unit
- Generator (Creates random detector data)
- Configuration for CODA



Courtesy of Dimitrios Arnellos

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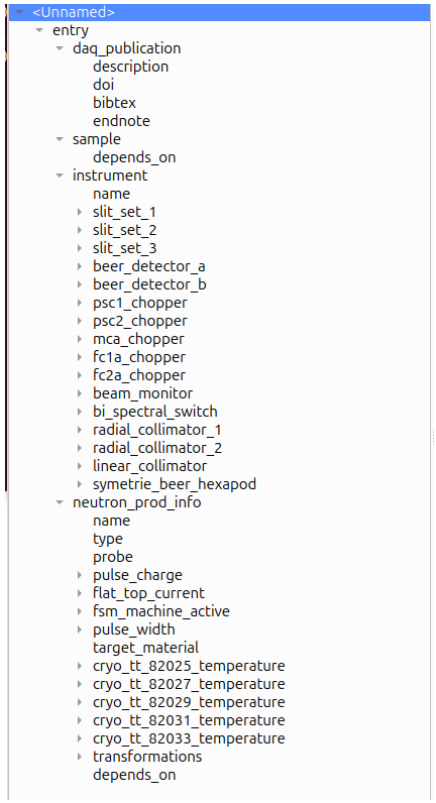

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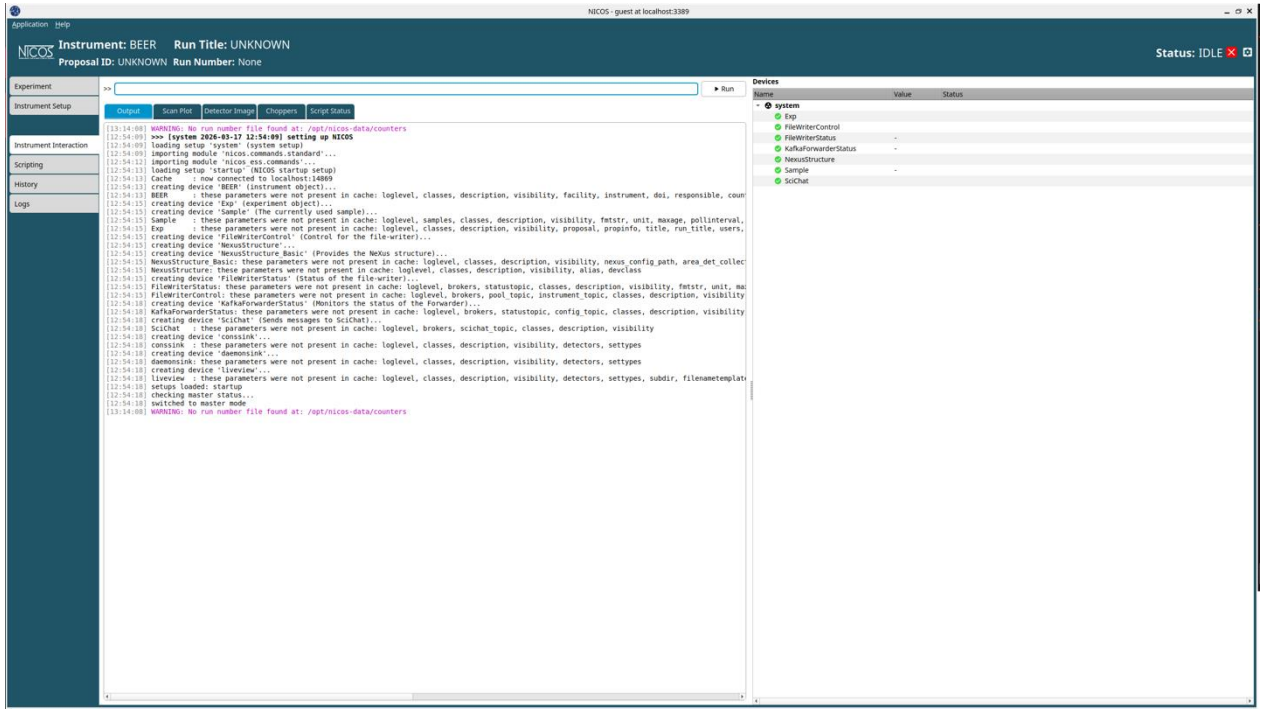
- NICOS (instrument control)

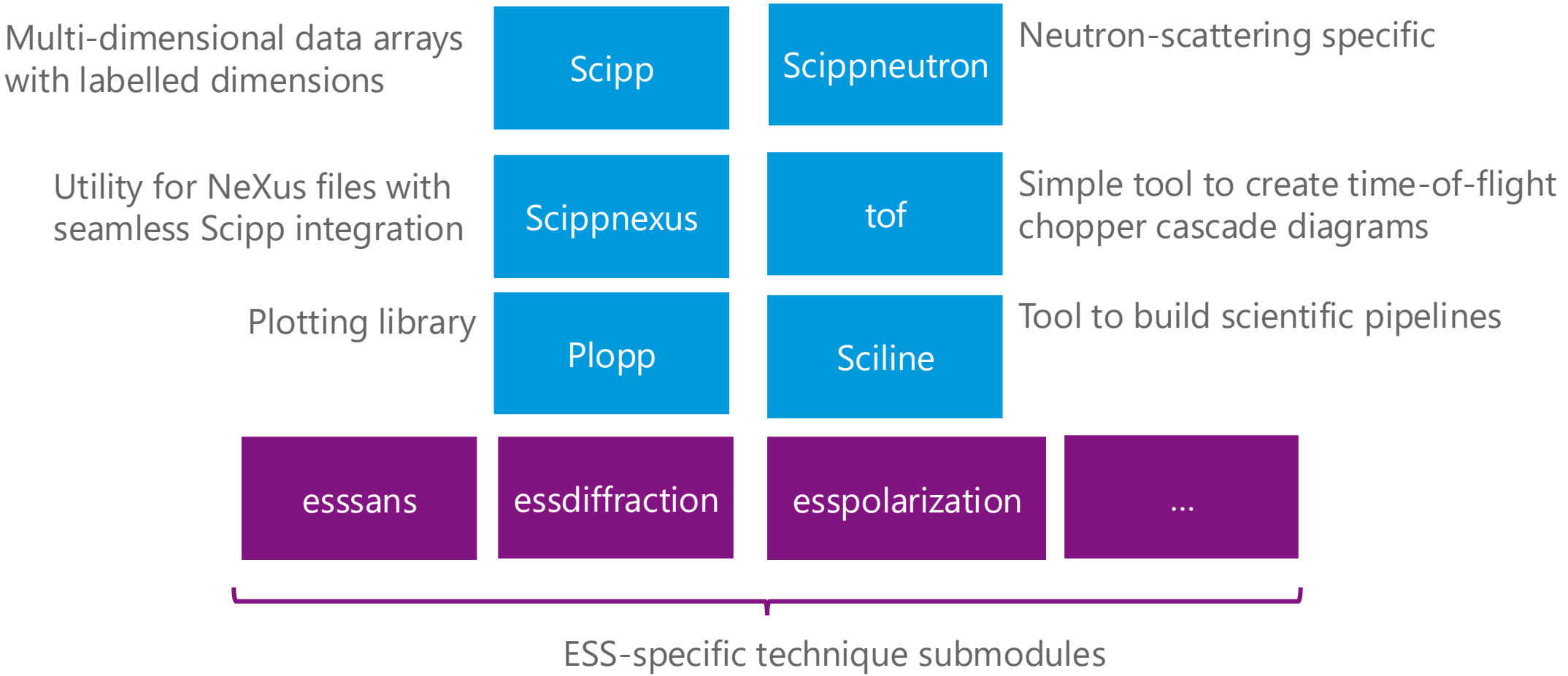
  - BEER NICOS Server provisioned
  - NICOS software deployed on server



Courtesy of Dimitrios Arnellos

Data reduction

Scipp – stack of frameworks

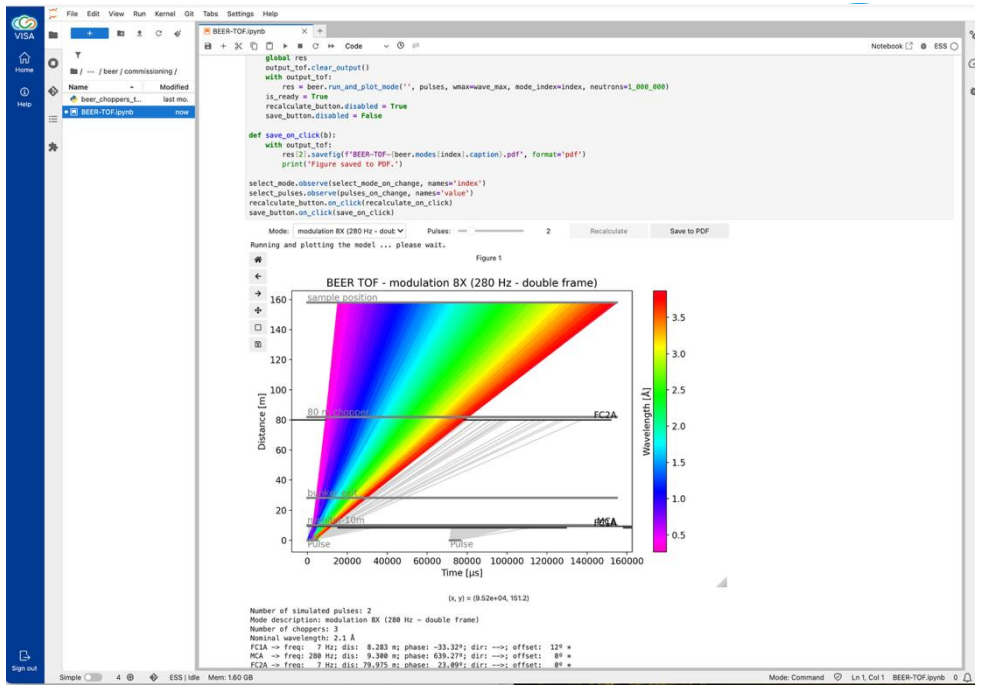


Data reduction

Scipp

Diagnostic tools

notebook from Premek available in Code Shelf



Data reduction

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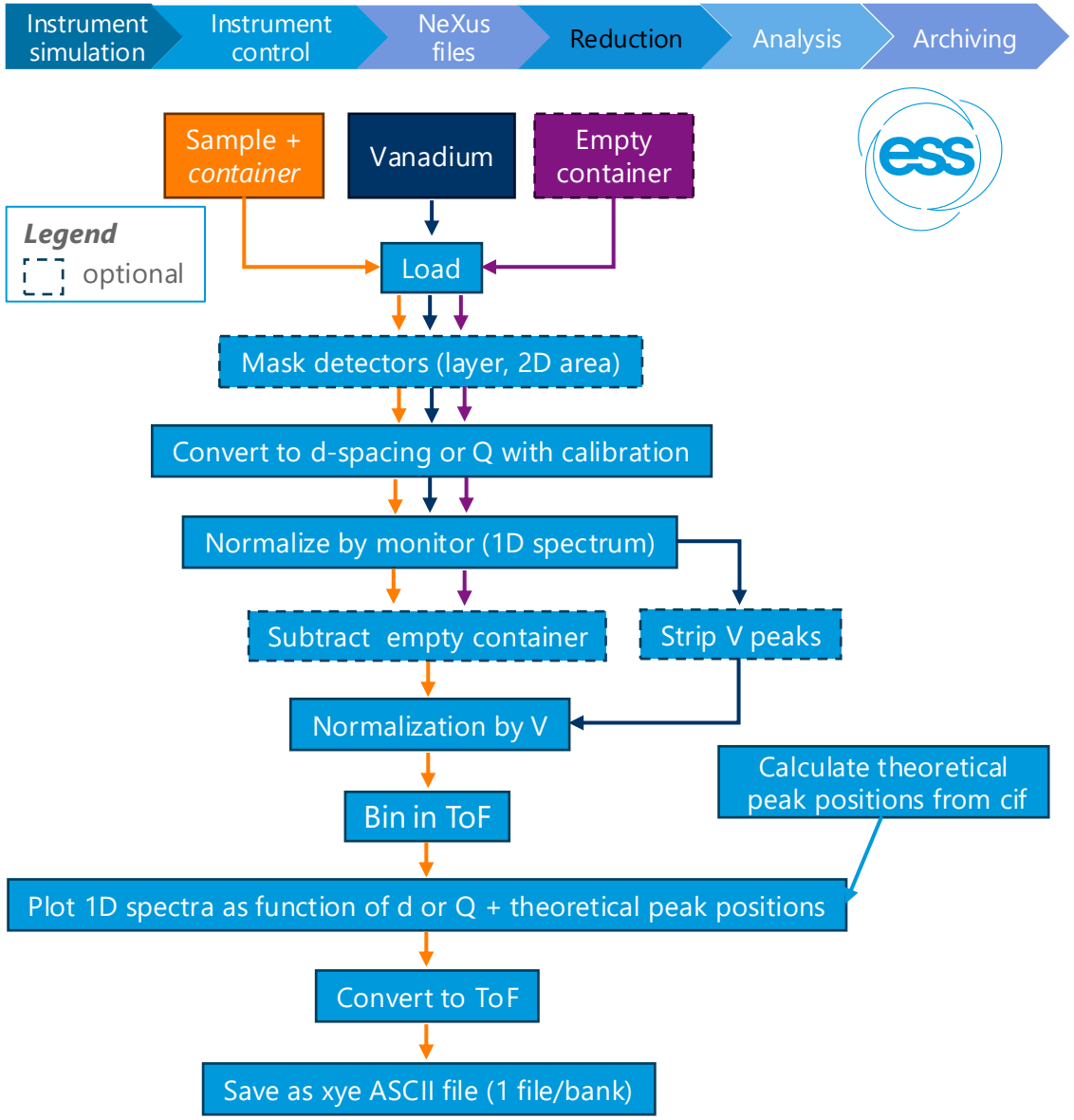
Features

- Loader for 3D detectors (McStas)
- CIF tools: extract peak positions from CIF using COD reference
- Powder diffraction workflow



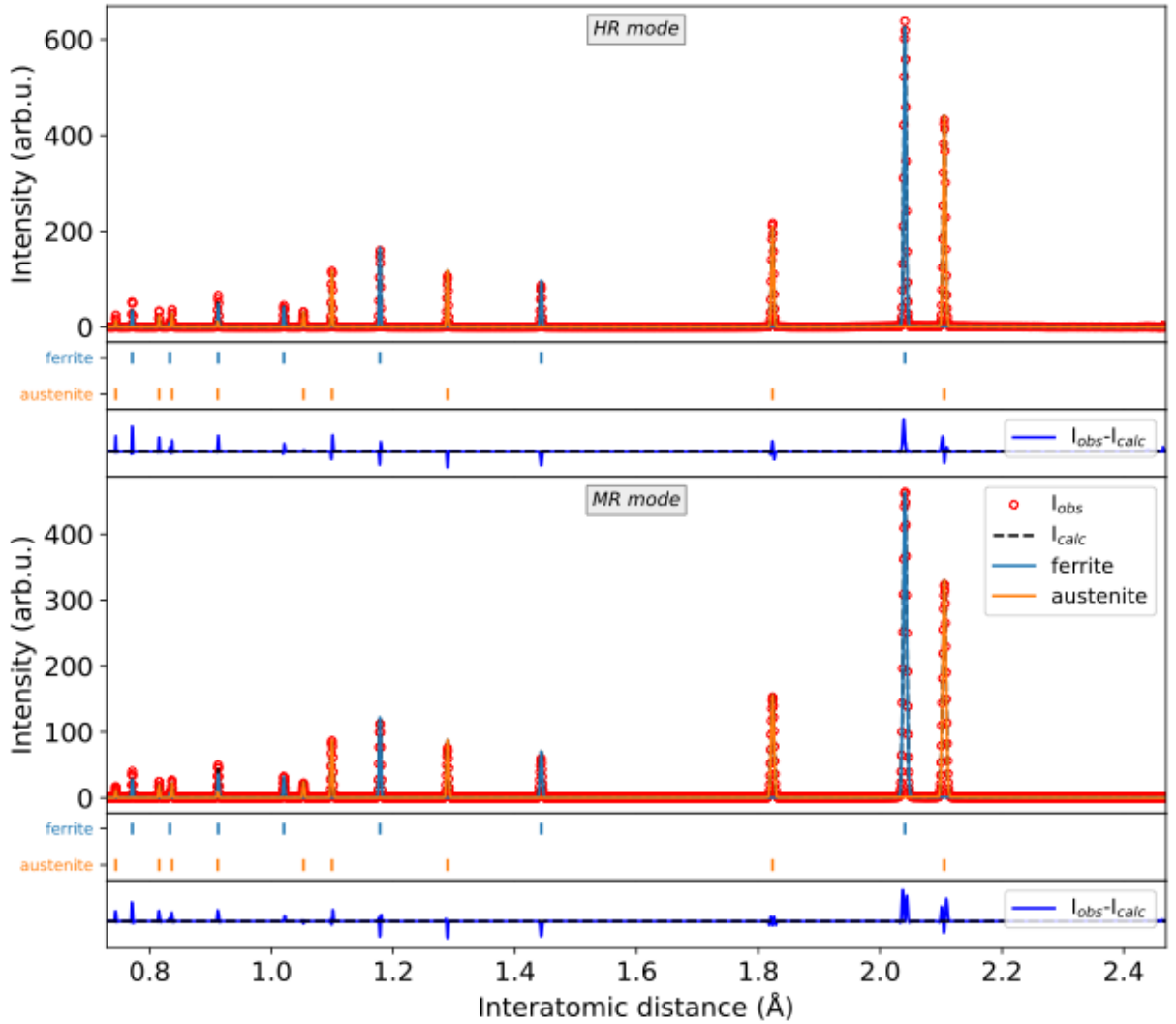
Data analysis

Simulation with Duplex steel – strain & microstrain analysis

- McStas simulation with 3D detector model
- High- and medium-resolution modes
- PowderN sample component with duplex steel sample (A:F – 50:50%)
- 4 mm collimators, sample r5, h20 mm
- Simulated homogenous lattice shift and RMS for microstrain
- Normalisation done to V sample
- Full pattern fitting using FullProf

Results

- Phase fraction: 50:50%
- Δd/d: 0.24 HR, 0.3 MR



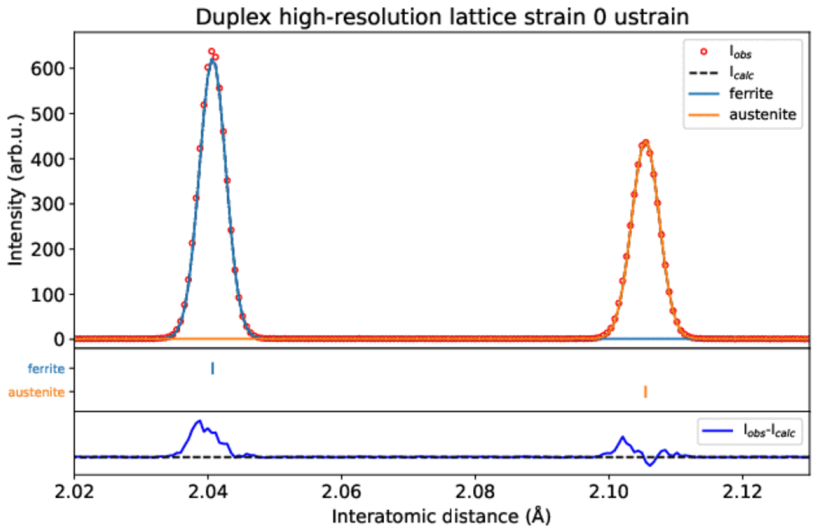
Data analysis

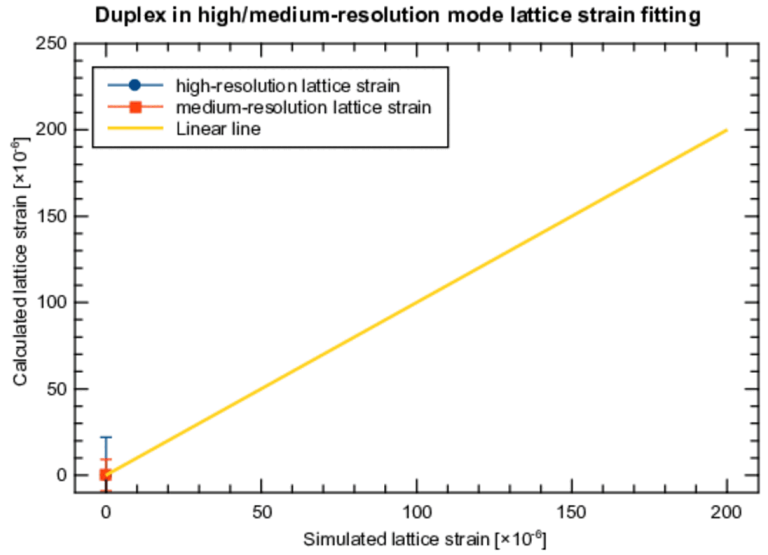
Simulation with Duplex steel – strain & microstrain analysis

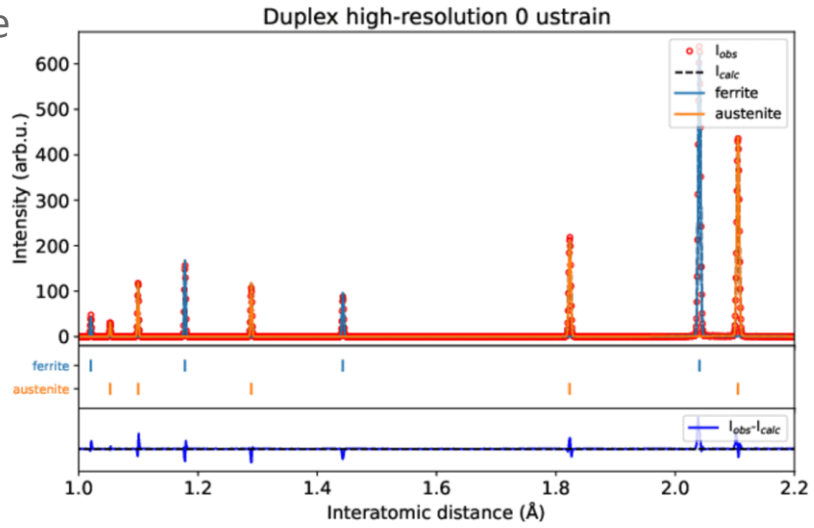
- Lattice strain from 0 to 200 µstrain with step 20 µstrain
- RMS strain from 0 to 5000 µstrain with various steps

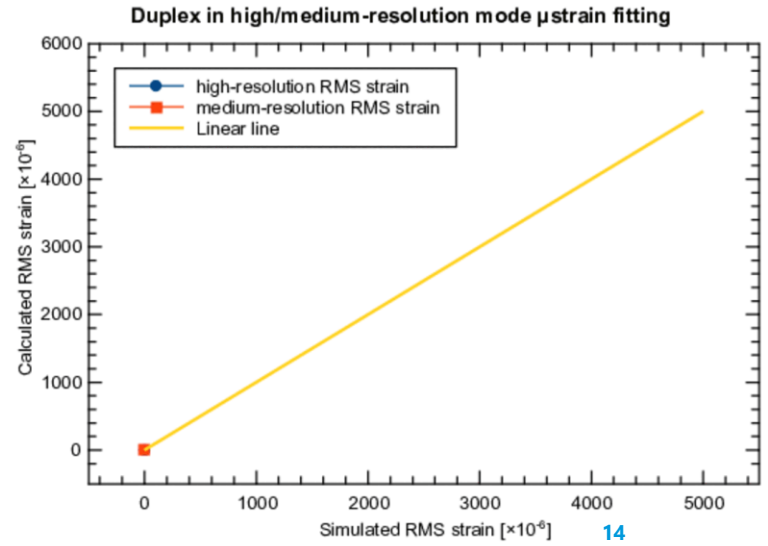
Results

- Reduction workflow works
- Analysed data correspond the simulated one
- Lattice/micro strain error bars: 10-20 µstrain









Data analysis

Various compositions to test normalisation

- Blind tests to verify the phase fraction evaluation ➜ all phase fraction analysed within 2 wt.%