The Data Reduction, Analysis, and Modelling group

Our role, activities and opportunities for collaborations

PRESENTED BY Mads Bertelsen
2023-10-05

EUROPEAN SPALLATION SOURCE

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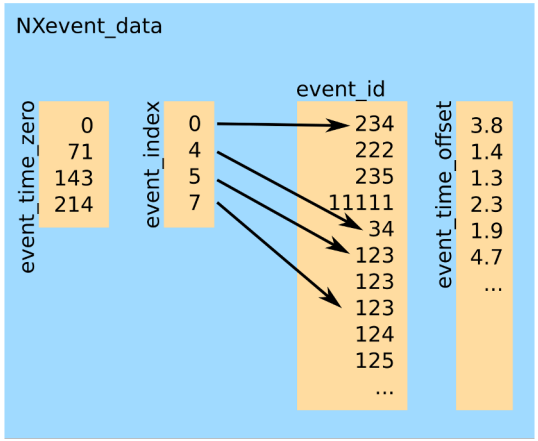
Data Reduction: convert detector data to physical data

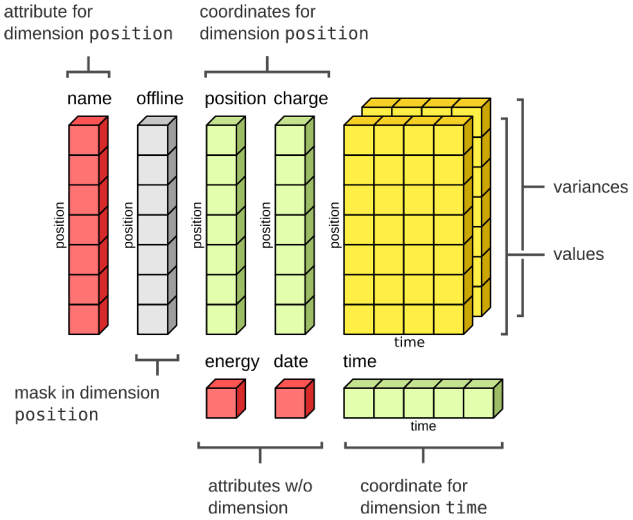
(pixel position, detection time) ⟹ (λ, energy, θ, d-spacing, intensity, …)

scipp

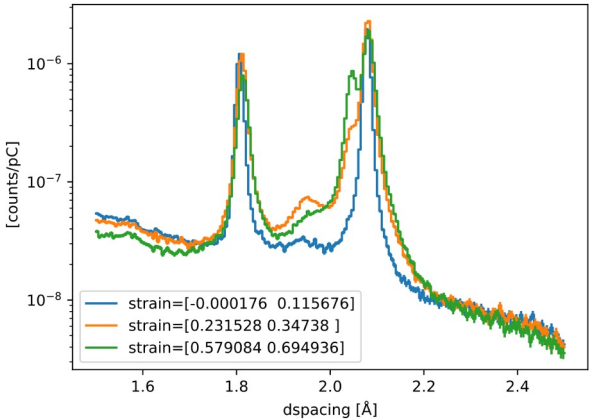
Event data in NeXus file



Scipp flexible data structure



Output with physical units

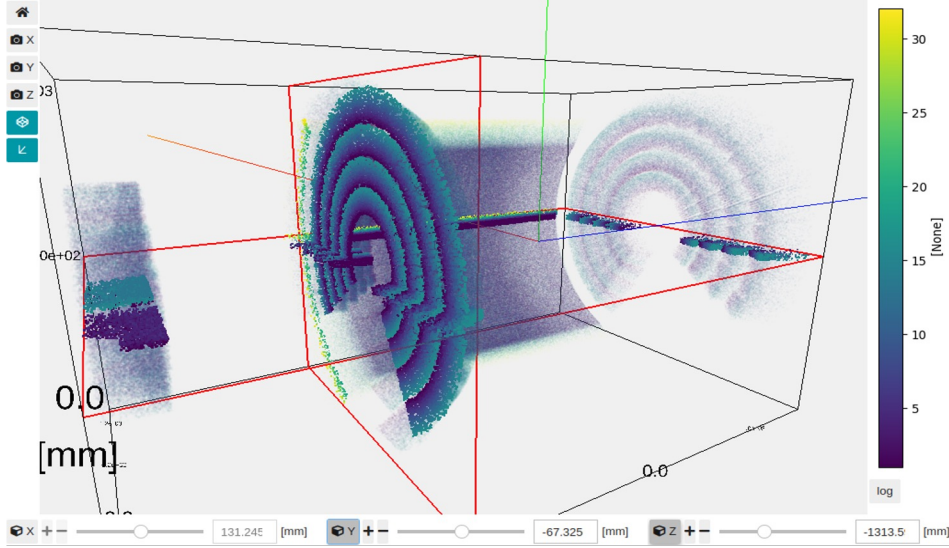


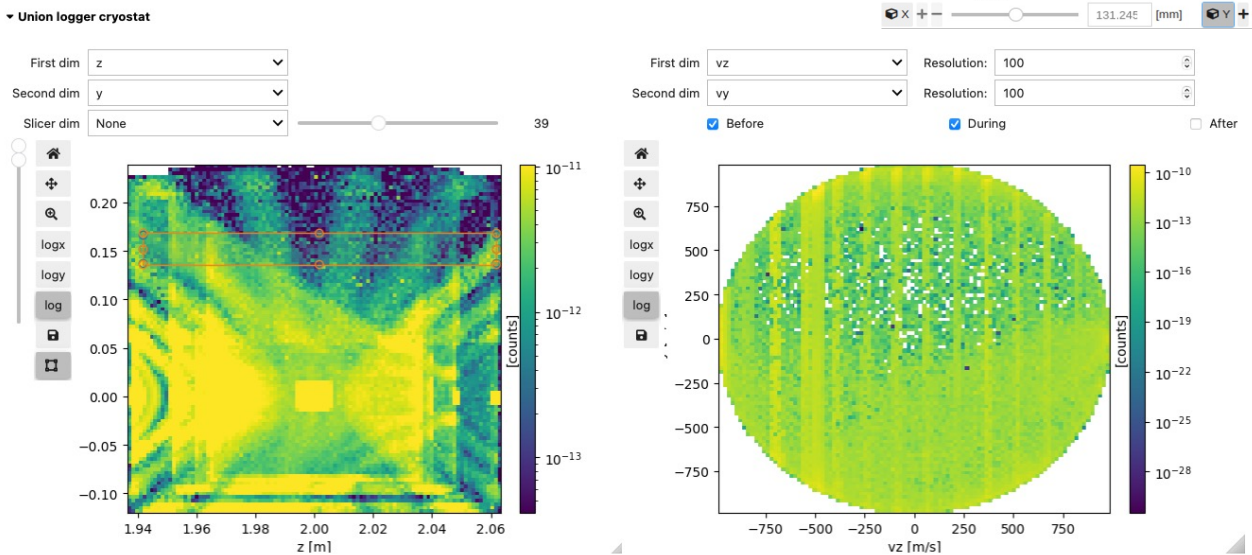
python™

scipp.github.io

Data Visualization

Interactive data visualization in Jupyter notebooks



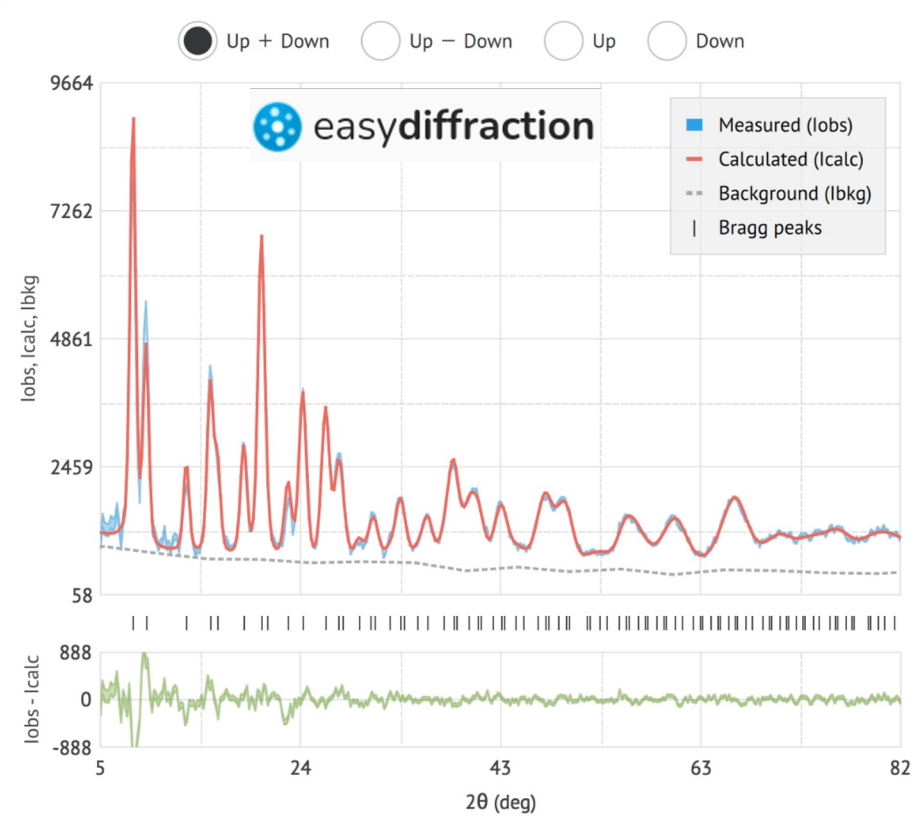


plopp

python™

scipp.github.io/plopp

Data Analysis: interpret and understand physical data



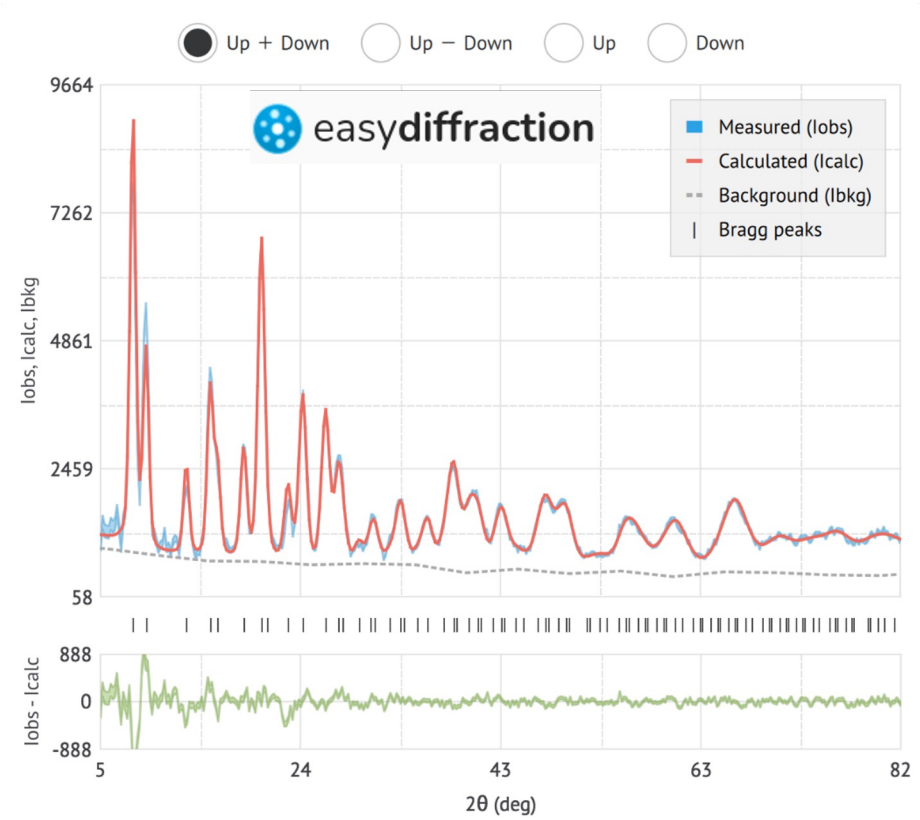
Parameters

No.	Label	Value	Error	Fit
1	**Ho2Ti2O7 cell length_a**	10.2659 Å	0.0009	✓
2	Ho2Ti2O7 **atom_site Ho occupancy**	1.0000 frac		
3	Ho2Ti2O7 atom_site Ho **U_iso_or_equiv**	0.0000 Å^2		
4	Ho2Ti2O7 atom_site Ho **susceptibility_chi_11**	3.8262 T^{-1}	0.0222	✓
5	Ho2Ti2O7 atom_site Ho **susceptibility_chi_12**	3.7380 T^{-1}	0.0154	✓
6	Ho2Ti2O7 atom_site **Ti occupancy**	1.0000 frac		
7	Ho2Ti2O7 atom_site Ti **U_iso_or_equiv**	0.0000 Å^2		
8	Ho2Ti2O7 atom_site **O1 fract_x**	0.3286 frac		
9	Ho2Ti2O7 atom_site O1 **occupancy**	1.0000 frac		
10	Ho2Ti2O7 atom_site O1 **U_iso_or_equiv**	0.0000 Å^2		
11	Ho2Ti2O7 atom_site **O2 occupancy**	1.0000 frac		
12	Ho2Ti2O7 atom_site O2 **U_iso_or_equiv**	0.0000 Å^2		

8.2127 — 12.3191

Start fitting

Data Analysis: interpret and understand physical data



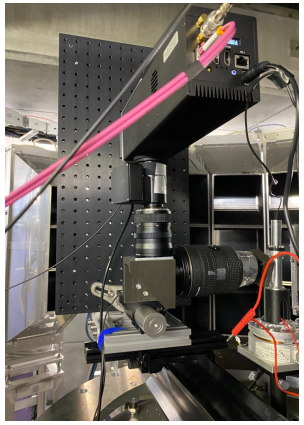
- Create strategy for analysis software for all planned instruments
- Involvement in neutron analysis software projects
- We actively work on ~20 open-source projects (our own initiatives, collaborative developments)

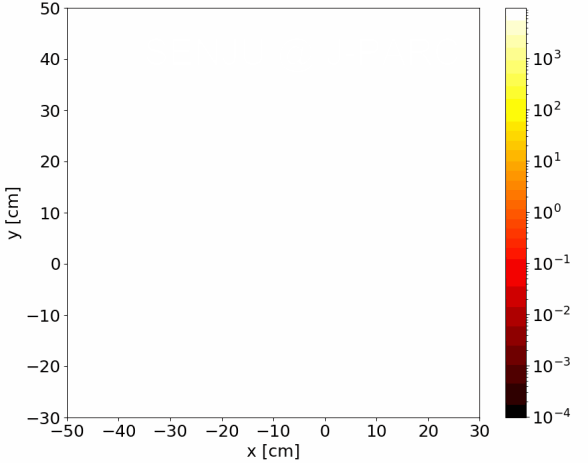
EasyDiffraction , EasyReflectometry , Brille , SasView , SpinW , CrysFML , CrysPy

python™ GitHub

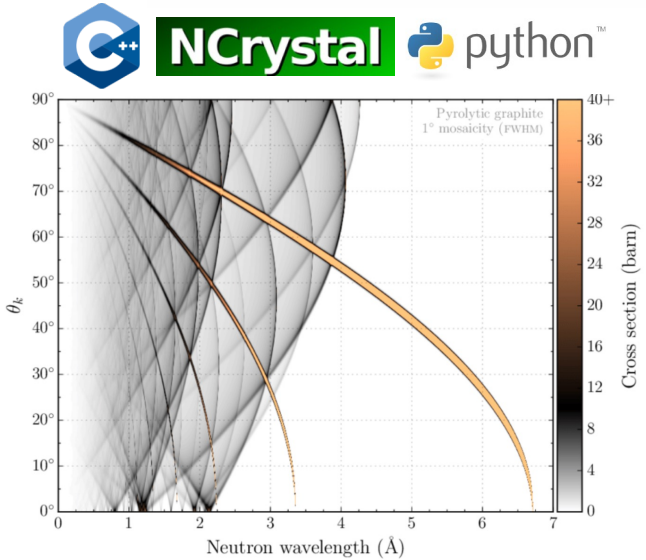
Modelling

- **Instrument simulation**:
  - McStas/McXtrace development
  - Instrument performance
  - Simulation of experiments

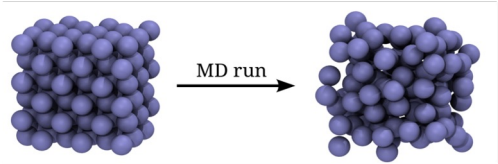




- **Neutron transport**:
  - Ncrystal development



- **Atomistic modelling**:
  - Use of DFT, MD, spin dynamics calculations for QENS and INS



Topic ideas for student projects

Rationale

Students can use newly developed capabilities for larger projects than the developers would have time for, with supervision from the developers. We see how potential users would use our software. Important feedback!

Topic ideas

- Data science: processing / manipulating / exploring large (sparse?) datasets
- Statistical analysis of experimental errors and propagations (Bayesian, correlations)
- Creating graphical user interfaces / Interactive data visualization
- User experience analysis / improvement of scientific software
- Applying machine learning to neutron science data reduction and/or analysis
- HPC (GPU computing) projects for MD & MC simulations

Examples of student projects

Student	Uni.	Project
Martin Olsen	KU	Coating optimization in neutron guides Cone and mesh geometry in McStas Union components
Petroula Karakosta	KU	Simulation of BIFROST magnet and machine learning (talk later)
Estrid Buhl Naver	DTU	Simulation of multilayer sample with refraction and reflections
Domenico Battaglia	DTU	Simulation of battery experiment at SENJU J-PARC

Recently started offering students desks at DMSC which have greatly improved collaboration

Thanks for your attention

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