SINE2020 General Assembly

Bilbao, May 2019

WP 10
Data treatment Software

WP leader:
Thomas Holm Rod, ESS ERIC

Presenter (ISIS WP10 facility coordinator):
Anders Markvardsen, STFC, ISIS

1. Objectives

- Straightforward generation of scientific results for non-expert and industry users using data treatment software

- Data treatment software ready for users at ESS in 2020

Advisor: Andy Götz, ESRF

Strategy

- Converge towards supporting the same software across facilities

- Enable users to leave facility with publishable results

- Facilitate automated data treatment workflows

- Enable 3rd party contributors to extend software

- Exploit and support modelling based on atomic-scale simulations

Tasks

- T10.1: Annual workshops + Meeting users

- T10.2: Standard & Guidelines (D10.1)

- T10.3: Mantid for continuous sources (D10.2)

- T10.4: Data analysis and modelling software (D10.3-8)

  (SasView, BornAgain, MuhRec, QENS/Mantid, MDANSE, abINS, QENSlib, MUESR+DFT calcs)

T10.1: WP10 Workshops

#WS	Org.	Date	Purpose	#Part
I	PSI	April, 2016	Kick off, coordination	26
II	ILL	April, 2017	Expert users, early adopters Deliverable 1	
III	MLZ	Spring, 2018	~~Broader user-commu~~ Deliverable 2-5	37
IV	ESS	Spring, 2019	~~Broader user-community~~ Deliverable 6-8	36

NOW

Delayed but delivered

On time

Budget for workshops: € 20,000

T10.1: Last workshop

Workshop IV (May 2019, ESS)

T10.1 Meeting the users

After Workshop II:

- Let WP10 workshops III & IV focus on developers (rather than users)
- Meet users where users are;

Software	Conference
SasView	XVII International Small Angle Scattering Conference (Oct. 2018) + schools
BornAgain	BornAgain School and User Meeting 2018 (Dec. 2018)
MuhRec / KipTool	11th World Conference on Neutron Radiography (Sept. 2018) + schools
MDANSE & abINS	MDANSE Summer School (Sept. 2019, Tenerife, Spain)
muons	2018 ISIS Muon School (March, 2018, Didcot, UK)

T10.2 Standards & Guidelines

Deliverable 10.1: Standards & Guidelines to basis for **collaboration** and development of **sustainable** software (STFC, due M18)

- Discussed in plenum at Workshop II

- Report with standards & guidelines accessible from sine2020.eu

- Being converted to peer-reviewed article

T10.3 Mantid for continuous src

- **Deliverable 10.2**: Converging on Mantid for continuous sources (ILL, due M30)

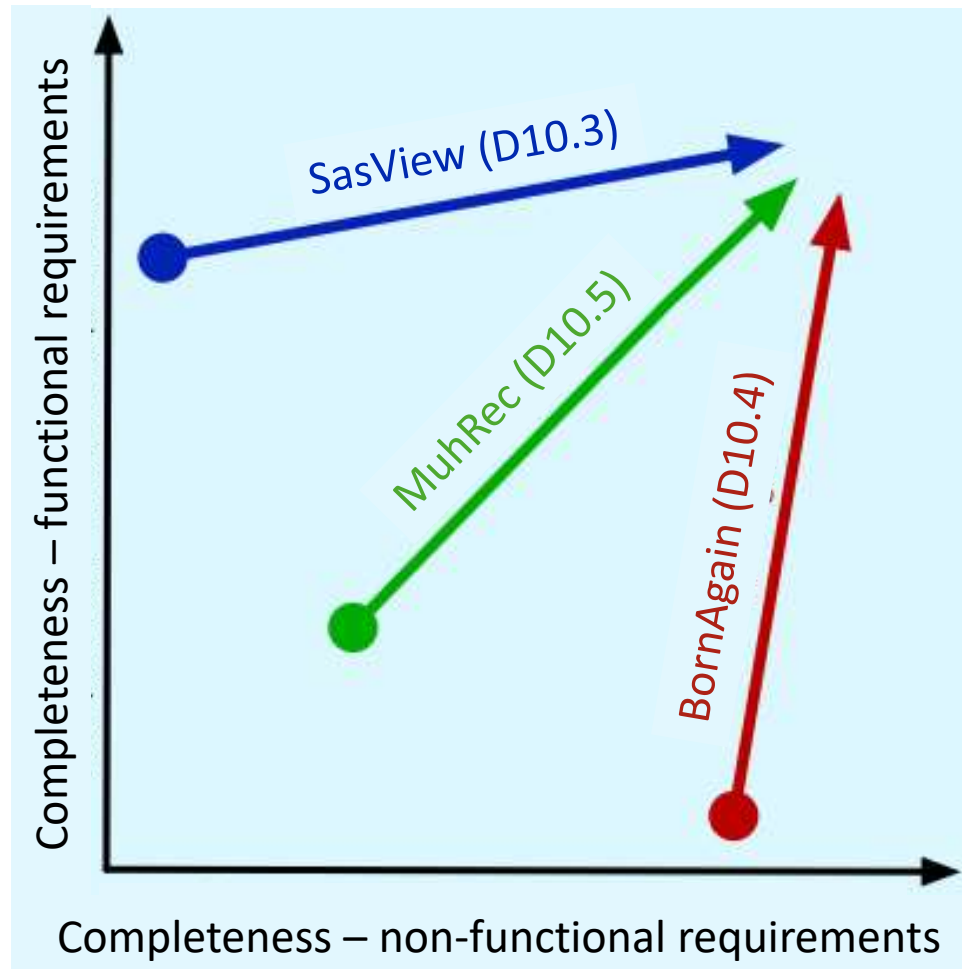| Facility	Instruments
ILL	D2B, D11, D17, D20, D22, D33, Figaro, IN4, IN5, IN6, IN16B
MLZ	TOFTOF, DNS, POWTEX (in construction)
PSI	AMOR, BOA, FOCUS, POLDI

- Additional resources from ILL

T10.4 Analysis and Modelling

Deliverable	Domain	SW Framework	Lead Facility
D10.3 + D10.8	SANS	SasView	ESS
D10.4 + D10.8	Reflectometry	BornAgain	FZJ/MLZ
D10.5 + D10.8	Imaging	MuhRec/KipTool	PSI
D10.6	QENS	Mantid + library	ILL, ISIS, ESS
D10.7	Atomic Sim.	• MDANSE • abINS • MUESR • DFT calcs for muons	• ILL • ISIS • UNIPR • UNIPR

T10.4: SANS, Reflectometry & img

Deliverable 10.3-5:
Software for SANS, reflectometry, and imaging ready for user testing

Different challenges:

Completeness – functional requirements

SasView (D10.3)

MuhRec (D10.5)

BornAgain (D10.4)

Completeness – non-functional requirements

T10.4: QENS & atomic simulations

QENS model library

- *Open source* & *interoperable*
- *Jupyter tutorials* using lmfit, Mantid, BUMPS for fitting

QENS GUI

- Requirements and discussions with potential users
- *Available* in Mantid
- *Demonstrated* at Workshop IV

MDANSE

- neutron scattering spectra from *MD simulations*
- Removal of technical depth

abINS

- **INS spectra from** *lattice dynamics*
- Developed from scratch

T10.4 muon spectroscopy

MUESR

- **Open source** & **interoperable** with Mantid

- Documentation added prior to 2018 ISIS Muon School

DFT calcs for muons

- DFT methods to predict the muon site

- **Training** in muon DFT techniques

Conclusions

- All deliverables (almost) delivered

- Demonstrating software for users at *scientific conferences* were successful

- SINE2020 has initiated *collaboration* between facilities

- SINE2020 has delivered *maintainable* and *inter-operable* software even beyond what have been funded by SINE2020

Beyond SINE2020

Discussion of *sustainability* at Workshop IV:

- The SINE2020 partners with scientific computing groups will be able to maintain software considered

- Will continue to have annual workshops

  - Update standard & guidelines

- Will discuss the opportunity to have MoU for software

Questions?

Deliverables

#Mo	Deliverable	#Works.
18	• Guidelines & Standards (D1)	II (ILL)
30	• Mantid and use case for continuous sources deployed (D2) • SasView, BornAgain, MuhRec+KipTool ready for user test (D3-5)	III (MLZ)
42	• Improved SasView / BornAgain / MuhRec+KipTool ready for user test (D8) • QENS and Atomistic simulation software ready for user test (D6,7)	IV (ESS)

NOW →

2. Work carried out

- ## Task 10.1 Dissemination and management

No	When	Venue	Deliverables	Desired participants
I	Spring '16	PSI		Involved partners
II	Spring '17	ILL	**D10.1** Standard & Guidelines	Expert users, early adopters,
III	Spring '18	MLZ	**D10.2** Mantid and use cases for continuous sources deployed. **D10.3-5** SasView, BornAgain, MuhRec/KipTool and use cases ready for user test	Broader user community
IV	Spring '19	ESS	**D10.6-8** QENS and atomic modelling software and use cases ready for user test	Broader user community

2. Work carried out

- **Task 10.1 Dissemination and Mng (continued)**
  - Workshop I @ PSI (KPI = 26 participants)

2. Work carried out

- Task 10.1 Dissemination and Mng (continued)
  - Workshop II @ ILL (KPI= 61 participants)

2. Work carried out

- Task 10.2 Standard & Guidelines (D10.1)
  - Work was led by ISIS (Anders Markvardsen)
  - Survey of software in WP plus McStas
  - Report (D10.1) presented and discussed at Workshop II
  - Agreed/confirmed S&G included: Open source, Python/C++/Qt etc

2. Work carried out

- Task 10.2 Standard & Guidelines (D10.1)
  - Also, standard for comparing fit minimizers
  - And improvement to how to document complex neutron data loaders

News

News and results related to th

Improving the fitting in Mantid for neutron and muon data

05/12/2016

2. Work carried out

- **Task 10.3 MANTID for continuous sources**
  - Continuous sources are ILL, PSI, and MLZ.
  - Existing Mantid members are ISIS, ESS, and SNS
  - Users will face same software (Mantid) at all involved facilities (KPI)
  - Also ILL in-kind contribution through Bastille
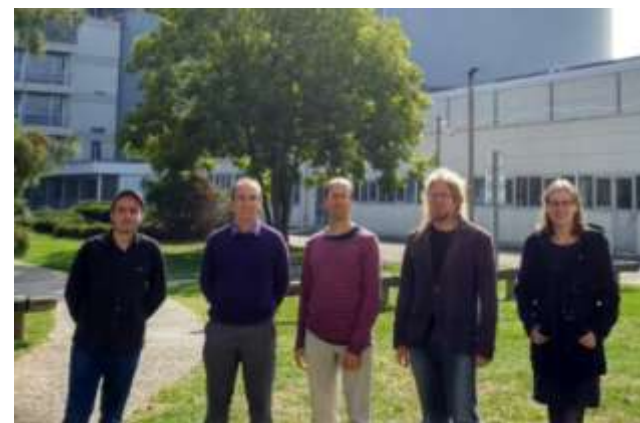
ILL team

PSI

FZJ/ MLZ

2. Work carried out

- Task 10.3 **MANTiD** for continuous sources

Status

Facility	Deployed on	In progress	Planned
ILL	IN16B, IN4, IN5, IN6	D17, Figaro, D1B, D2B, D20	D4C, D7, D16
PSI		AMOR, BOA	
FZJ/MLZ	TOFTOF	DNS	TOPAS, PowTex

D10.2: Mantid and use cases for continuous sources deployed
KPI: Numbers of facilities employing software from this WP
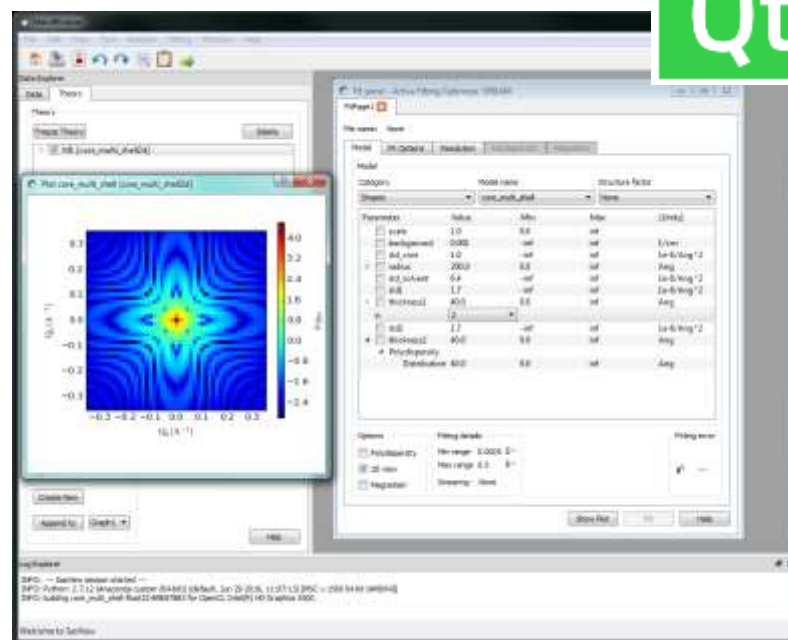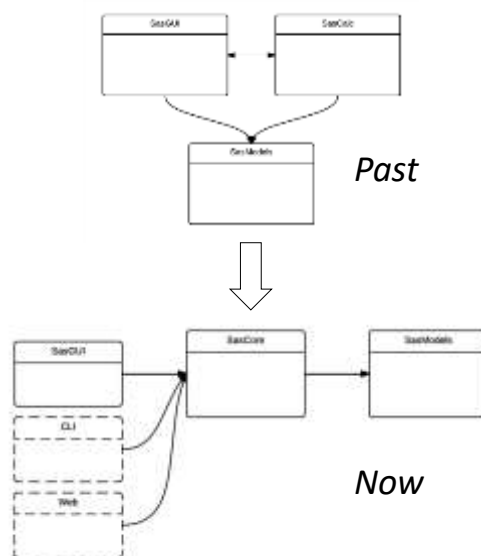
2. Work carried out

- Task 10.4 Interoperable data treatment SW

| Domain	SW Framework	Facility
SANS	SasView	**ESS**
Reflectometry	BornAgain	**FZJ/MLZ**
Imaging	MuhRec/KipTool	**PSI**, LLB, ESS (HZB, DTU, TUM, TUD)
QENS	Mantid?	**ILL,** ISIS, ESS
Muon spect.	Mantid (+ASE?)	**UPARM**, ISIS
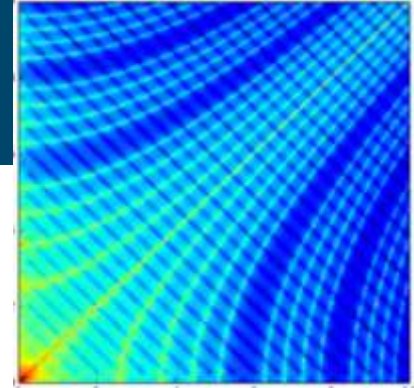
BornAgain for reflectometry

- Fairly new code (Version 1.7)
- Complies with our technical standards (Python/C++/Qt)
- Developed by FZJ/MLZ scientific computing group
- Designed for GISAS
- Not widely used for conventional reflectometry
- GUI still needs development
- First deliverable coincides with Workshop III

FZJ/MLZ BornAgain team
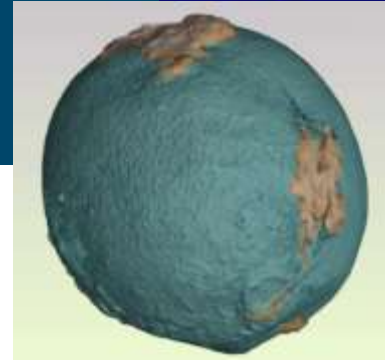
MuhRec/KipTool for Imaging

- Huge interest in contributing:

  - **PSI**, LLB, ESS, TUD, DTU, HZB, TUM

- Programs developed by Anders Kaestner

  - Single-point-of-failure

  - 'Closed source' -> Open source

- Python/C++/Qt with little technical debt

- First deliverable coincides with Workhop III

- LLB (F. Ott) contributes with algorithms

- ESS (A. Fedrigo) contributes with build servers and x-ray/neutron data fusion

- ISIS (F. Montesino & D. Tasev) tested MuhRec and worked on using it with existing software

PAUL SCHERRER INSTITUT
PSI

Comparing challenges

Software	Positive	Challenges
SasView	Wide spread usage and support	Technical debt
BornAgain	No technical debt Supported by SW engineering group	Not widely used for reflectometry
MuhRec/ KipTool	Little technical debt	Single-point-of-failure Lack of SW dev. infrastructure Documentation

Muon spectroscopy

- Muon spectroscopy is a complementary technique to neutrons

- Collaboration between Univ. of Parma and ISIS (ISIS: A. Lim, S. Cottrell, A. Markvardsen)

- Goal is to develop analysis software for muon spectroscopy

  - based on DFT calculations
  - Using Mantid as framework
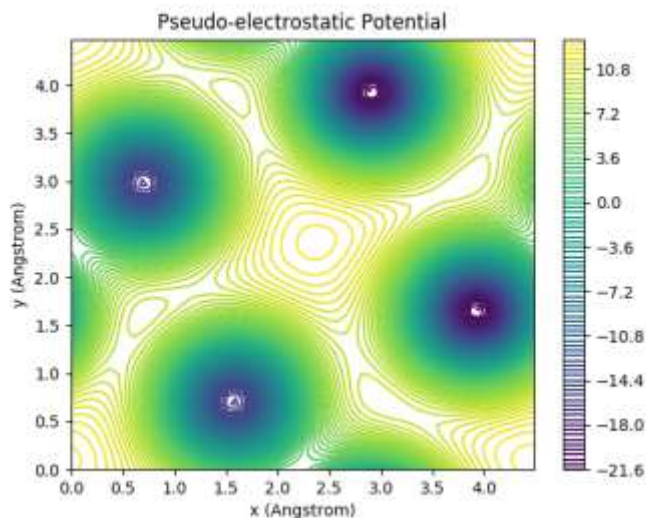
- Synergies with neutron scattering
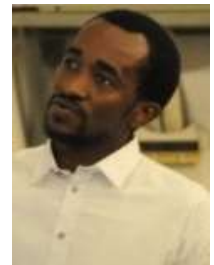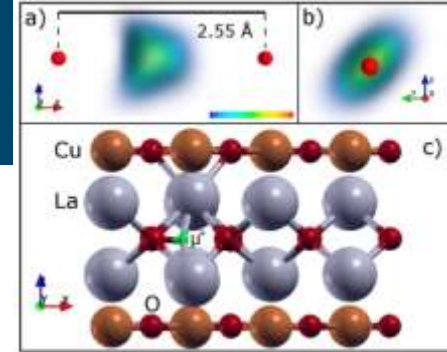
ASE mini-codecamp

- ASE is an interface to atomic-scale modelling software (e.g. DFT)

- Is ASE a useful tool for us?

GPAW tutorial

ASE mini-codecamp at ESS in Copenhagen

3. Impact

■ Increased awareness in community of the importance of having sustainable software

■ Improved collaboration and sharing of efforts based on shared values

■ Sharing of expertise and best practice across facilities

■ Training of scientists in `best practice` software development. Skills applicable in both academia and industry.

■ Other (non-project) partners also contribute now when they can see a significant concerted effort

4. Deviations / Problems encountered

- No delays so far

- It may be hard for a scientific computing group to convince instrument teams to use software supported by this project if they already use different software.

    - Envision that this issue will diminish as more and more people see the benefit of the project
    - There should still be space for other software

WP10 Objectives

- Straightforward generation of scientific results for non-expert and industry users …

- Data treatment software ready for users at ESS in 2020

Strategy

1. Converge towards supporting the same data treatment software at all facilities

2. Make it possible for users to leave a facility with analysed data and publishable results

3. Facilitate automated data treatment workflows

4. Make the software extensible and open for 3rd party contributions

5. Support atomistic simulations in order to nurture high impact science.

Workshop I, PSI, Spring 2016

Workshop II, ILL, Spring 2017

Workshop III, Sorogna, Spring 2018

Schedule for Workshop IV

	Wednesday @ Lundia	Thursday @ ESS	Friday @ Lundia
Morning	Site tour Registration	Site tour & Break out sessions (e.g. refl GUI, format for reduced data, etc)	Sustainability
Noon	Lunch @ Lundia	Lunch @ ESS	Lunch @ Grand
Afternoon I	Project Status Deliverables 3-8	UX & GUI (front end)	
Coffee	Fika	Fika	
Afternoon II	Project Status	Development	
Evening	Dinner @ Lundia	Dinner @ Grand	

Practical details

- Topics for discussion at breakout sessions to be decided at the end of today. We have X meeting rooms available plus open space outside Brightness and lunch space

- Group photo tomorrow at 15:10 at Horizon viewing platform

- Transport to and from site:

  - Morning to site: taxis

  - Afternoon back to hotel: Bus line 20

- For site tour: Only long pants are allowed (can be borrowed)

- Other things: Ask Danielle!

Deliverables

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Sustainability

1. **How do we ensure continuous collaboration & alignment?**

2. **How do we continue to maintain software considered in SINE2020?**

   - Annual workshops?

   - How do we keep standard & guidelines updated and relevant?

   - What about diffraction and spectroscopy?

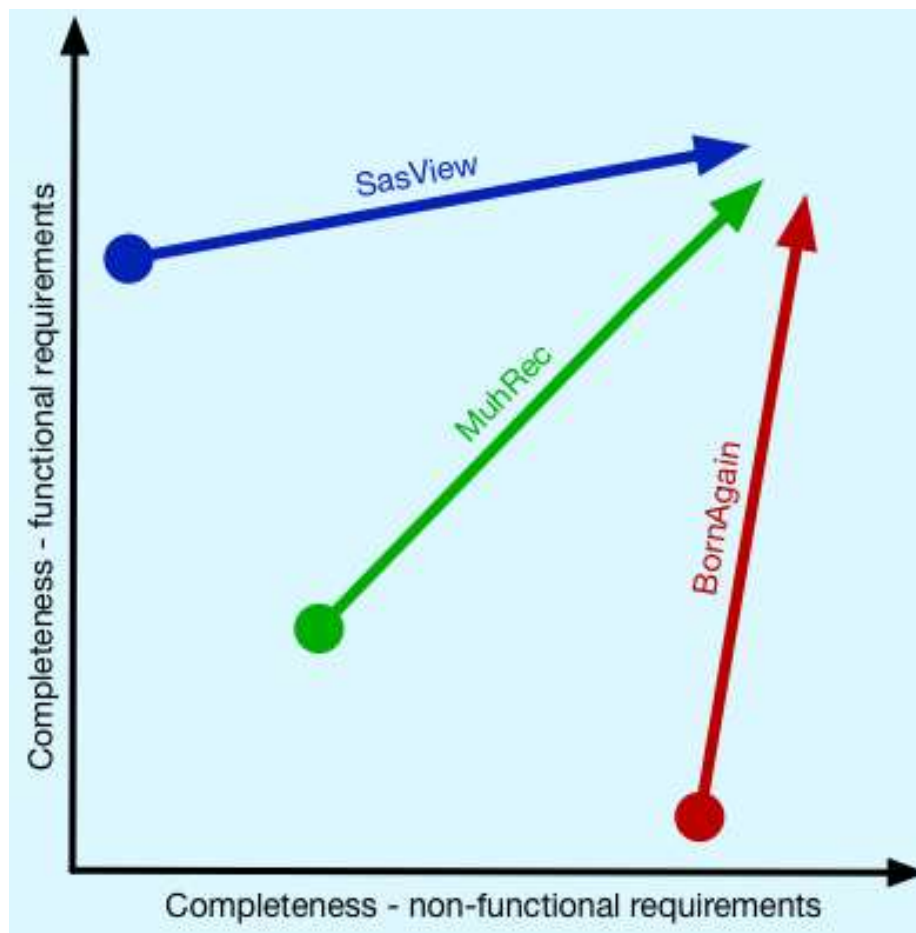# Deliverables

Standard & Guidelines

- Report -> paper
- Common base for open collaboration
- Almost all software considered in SINE2020 almost adhere to S&G

Mantid for continuous sources

Purpose: Users face same software at all facilities – easier to get acquainted with ESS

Result: Mostly ILL (additional resources)

Analysis SW: different challenges

+ **QENS lib**
+ **QENS GUI**

Atomic-scale simulations

- AbINS (new, embedded in Mantid)

- MDANSE (removing technical debt)

- Muon spectroscopy (DFT and muesr)

Feedback to advisory committe

- While WP10 was strongly promoted by the Head of Facilities, SINE2020 does not seem to be ingrained in any strategy at the respective facilities (with the exception of ESS).

Explanations of the work carried out

1. Objectives
2. Work carried out so far
3. Expected impact
4. Deviations / Problems encountered