

ESS facility news and update

Jon Taylor

Mantid User Meeting
ORNL 29 January 2018

Where is my data?



How do I get it?

How do I look at it?

What does it mean?



European spallation source



**High power long pulse spallation neutron source
The brightest source of cold neutrons worldwide
Incident flux $\sim 10^7\text{-}10^{10}\text{ n/s/cm}^2$
New scientific possibilities**



European facilities landscape



- **10 photon sources**
- **7 neutron sources**
- **Represents ~40 000 users/year**
- **PaN is not CERN**



Construction progress

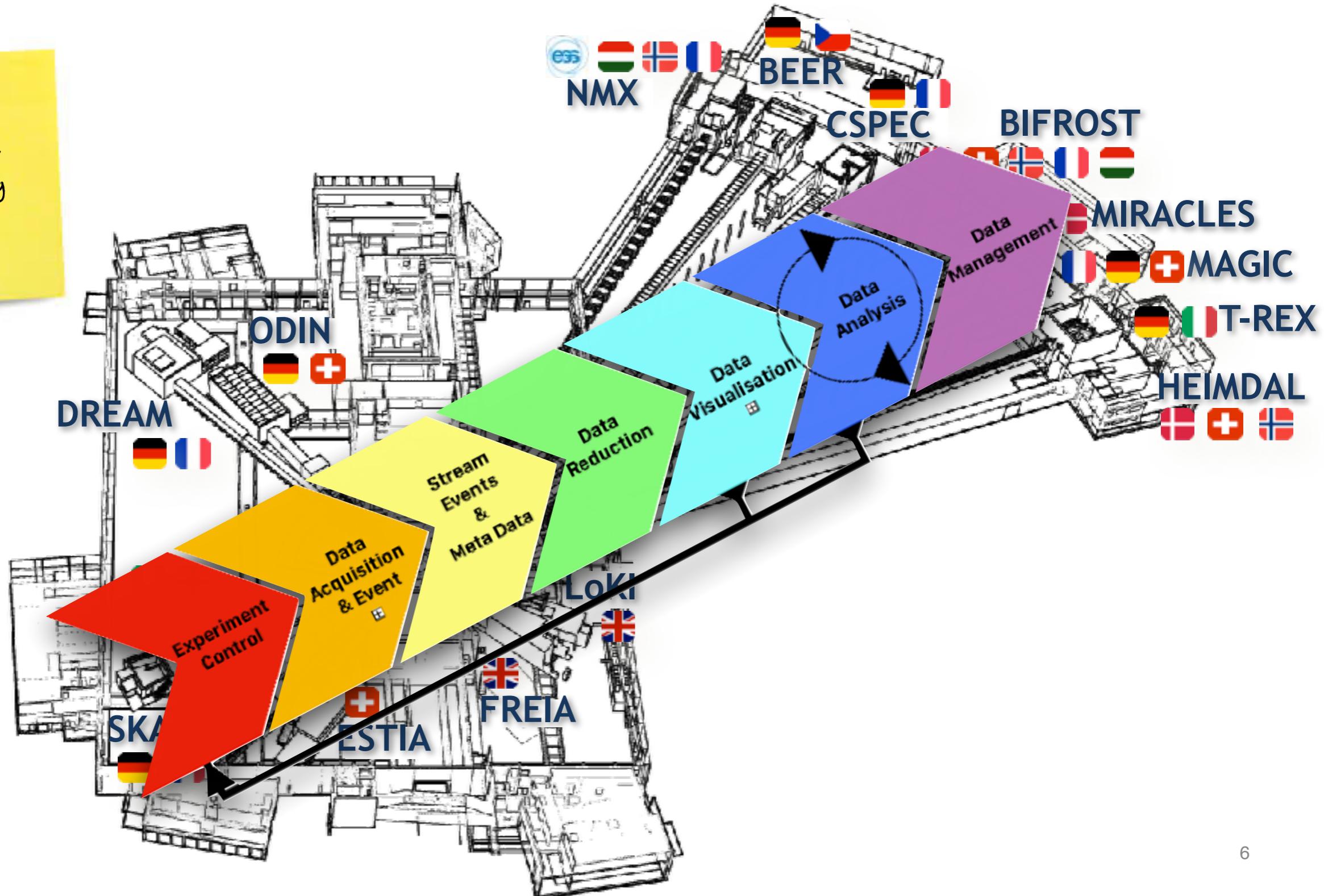


40 % complete

Accelerator installation started

14 instruments in detailed design

TO DO:
Scientific
computing
for this



Data Management and Software Centre



Provide world leading scientific software and scientific computing support for neutron scattering at ESS

- Construction budget 20M euro
- Staff 2018 27 + 8
- Staff 2028 60

Scientific Software development.

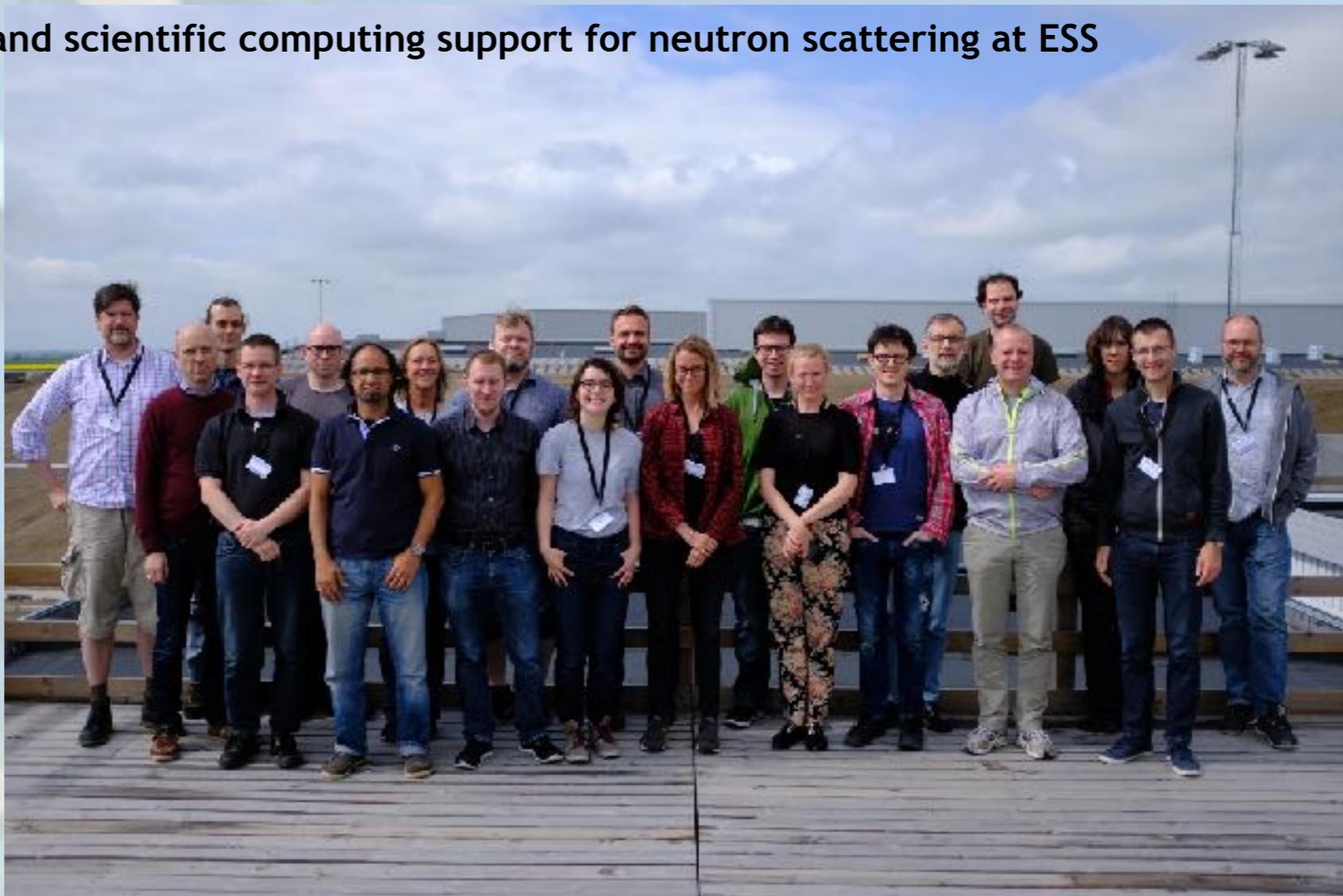
- Experiment control
- Data acquisition system
- Data reduction, analysis & modelling

Data centre operations.

- Dual location - Lund & Copenhagen
- Data management and curation

User programme support

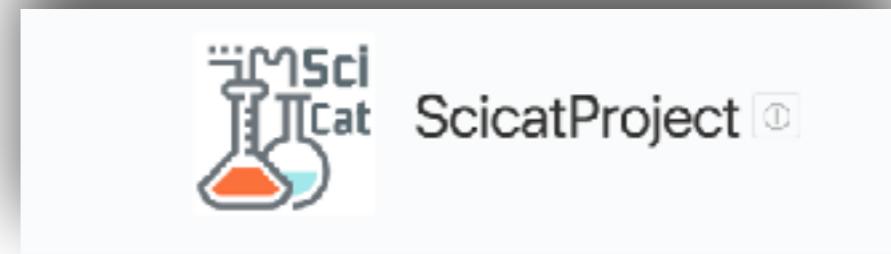
- Instrument Data scientists
- User office software
- Remote access to data and software tools



Policies and Projects



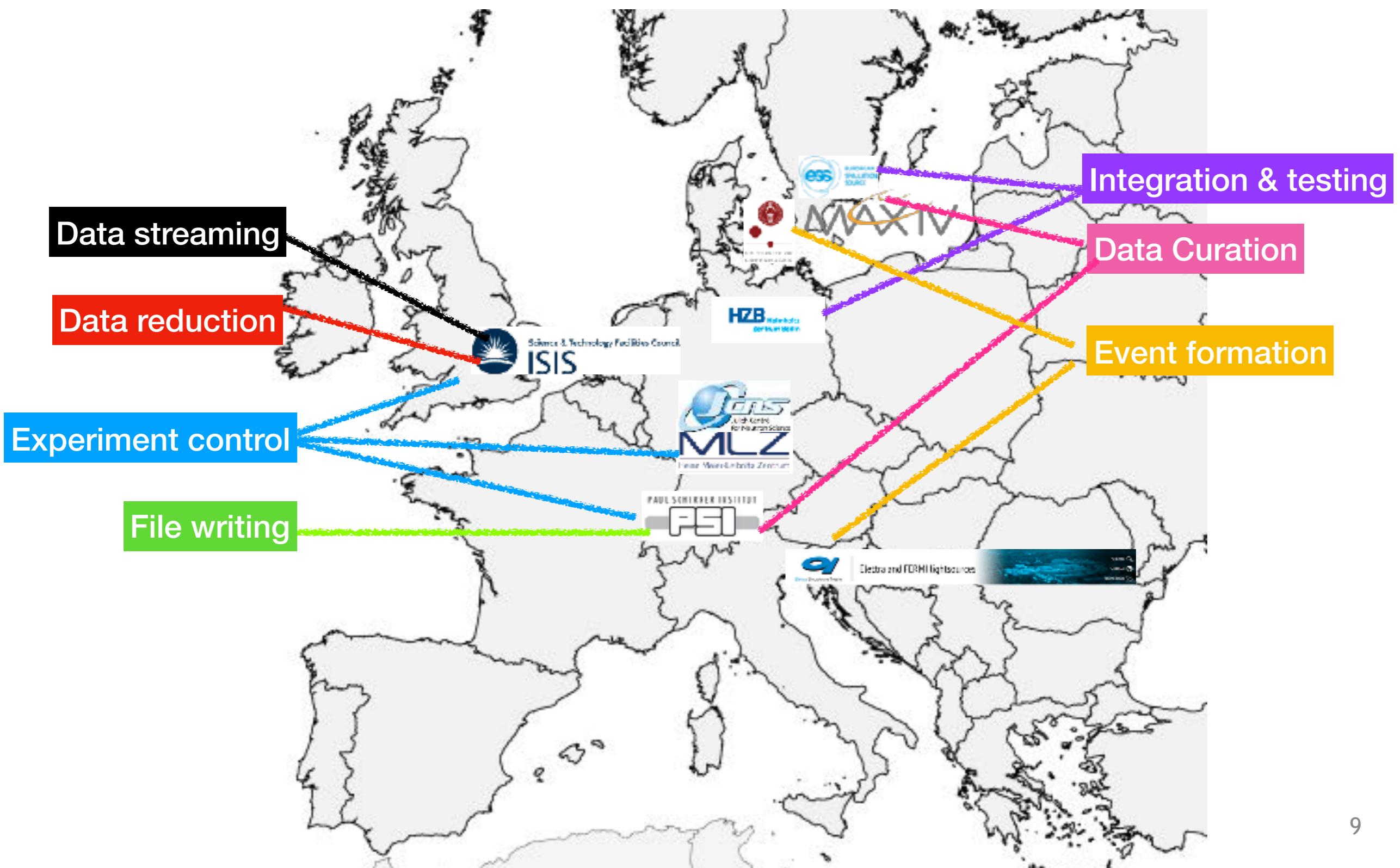
A screenshot of a document page from the European Spallation Source (ESS). The header includes the ESS logo and the text "EUROPEAN SPALLATION SOURCE". The document title is "Policy for Scientific Data". The footer contains the ESS logo and document metadata: "Document Identifier: CHSS Controlled Core", "Date: Mar 12, 2024", "Revision: 2 (P)", "Status: Released", and "Page: 1 (G)".



A screenshot of a document page titled "ESS INSTRUMENT SOFTWARE PROJECTS AND SOFTWARE PROJECT GOVERNANCE". The header includes the ESS logo and document metadata: "Document Identifier: CHSS Controlled Core", "Date: Mar 12, 2024", "Revision: 2 (P)", "Status: Released", and "Page: 1 (G)".



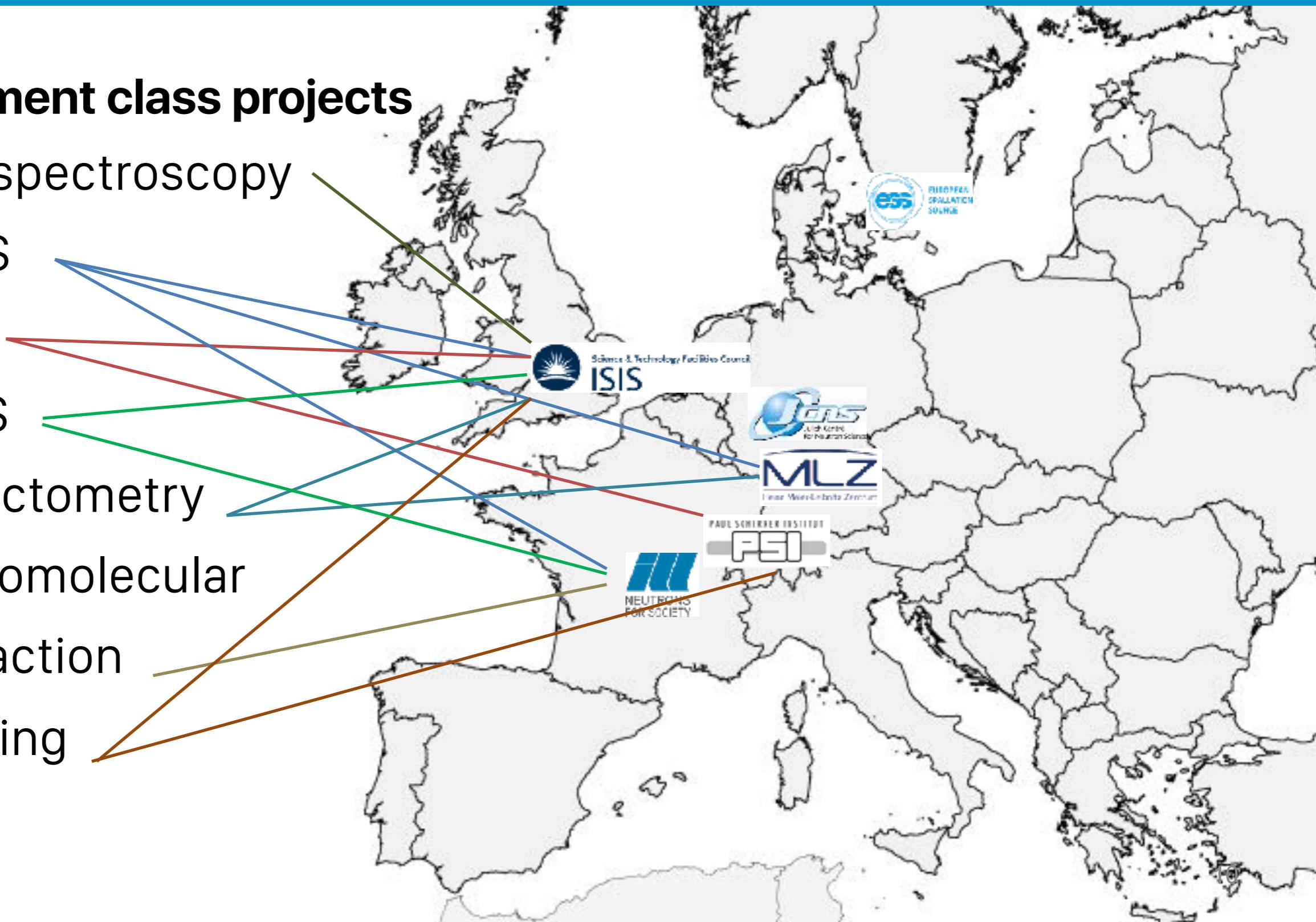
European collaboration ensures *maintainable* software for core instrument software



European collaboration ensures *maintainable* software for all instrument classes

Instrument class projects

- Mol. spectroscopy
- QENS
- INS
- SANS
- Reflectometry
- Macromolecular
- Diffraction
- Imaging



DMSC Collaboration With MAXIV



Objective : A single user portal for P&N in Lund

User Office working group

- ESS: Tobias Richter, Henno Gous, Arno Hiess, Sune Bahn
- MAXIV: Darren Spruce, Fredrik Bolmsten,

Current activities and progress

- Architecture development begins 2018
- Currently hiring an IT Architect in progress,
 - **first interviews will take place in week of Nov 27.**
- Solution / Framework candidates have been analysed
- High level requirements initially documented are being revised
- Architectural decision under review
- <https://confluence.esss.lu.se/display/DMSC/Architecture+for+user+office+software>

Next 6 months

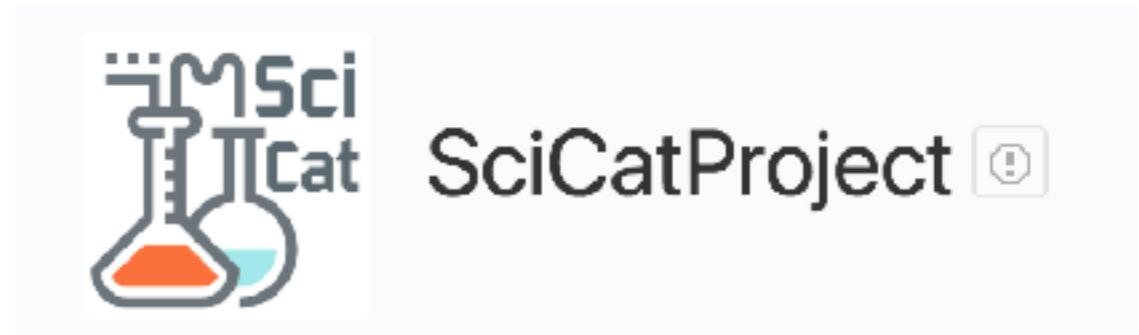
- Hiring and on boarding of IT-Architect to act as ESS project lead
- Establish a stakeholder group/steering committee (including beam line scientists / responsibles)
- Detailed planning
- Decide on solution/framework

DMSC Collaboration With



Objective: Common Data Curation & Management for MaxIV and ESS

- Common metadata catalogue for neutron and photon data to support principles of FAIR data
 - (Findable, Accessible, Interoperable, Reusable)
- Developed using modern web development framework for flexible and customisable display of domain specific metadata
- Active Open Source development.
- Prototype running at one SLS beamline in PSI
- Test deployments to be rolled out at MAX IV and DMSC
- Partners:
PSI (in kind to ESS) — Stephan Egli & Chris Gwilliams
DMSC — Gareth Murphy & Tobias Richter
MAX IV — Fredrik Bolmsten, Darren Spruce, Sair Quaderi, Hannes Petri



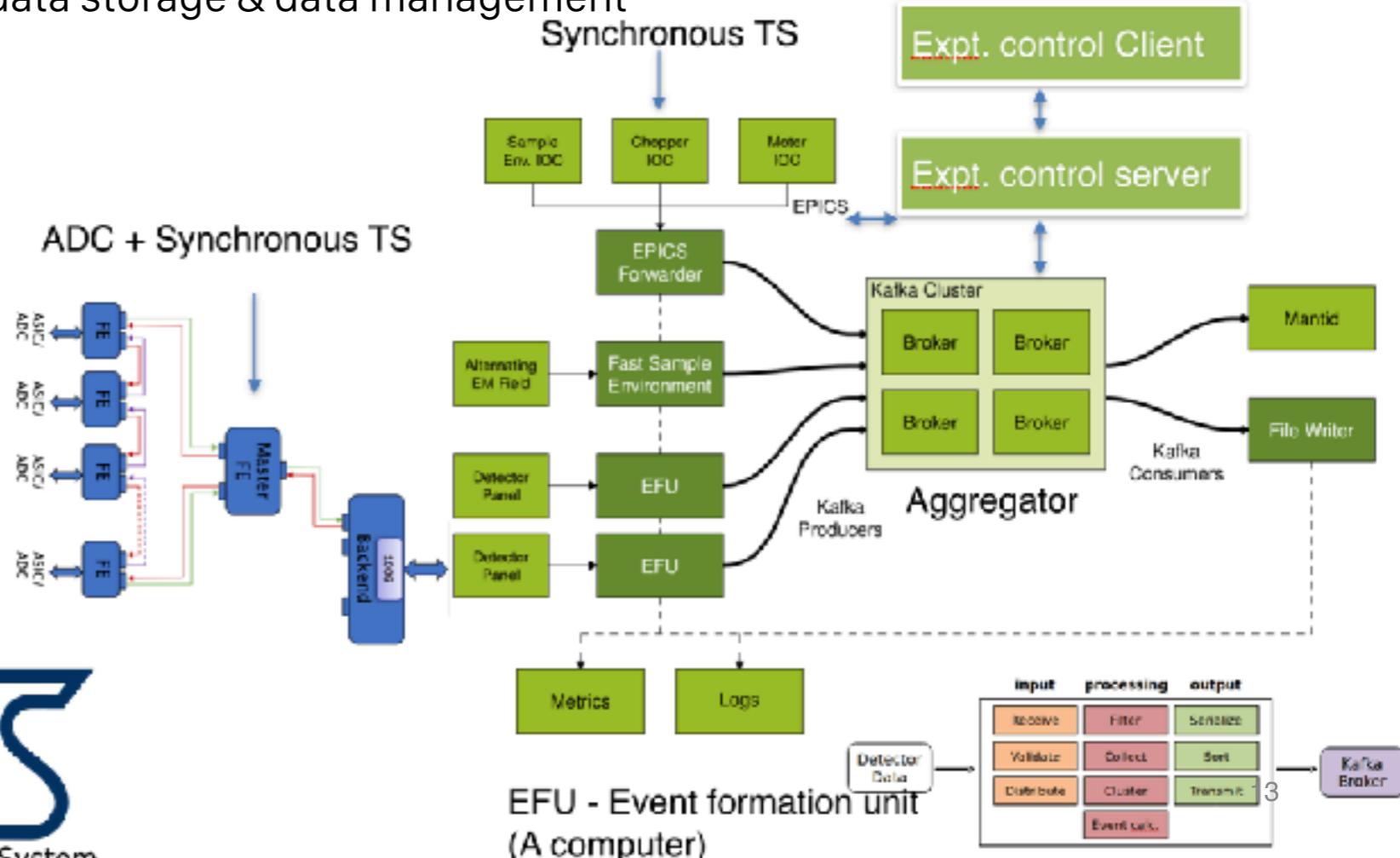
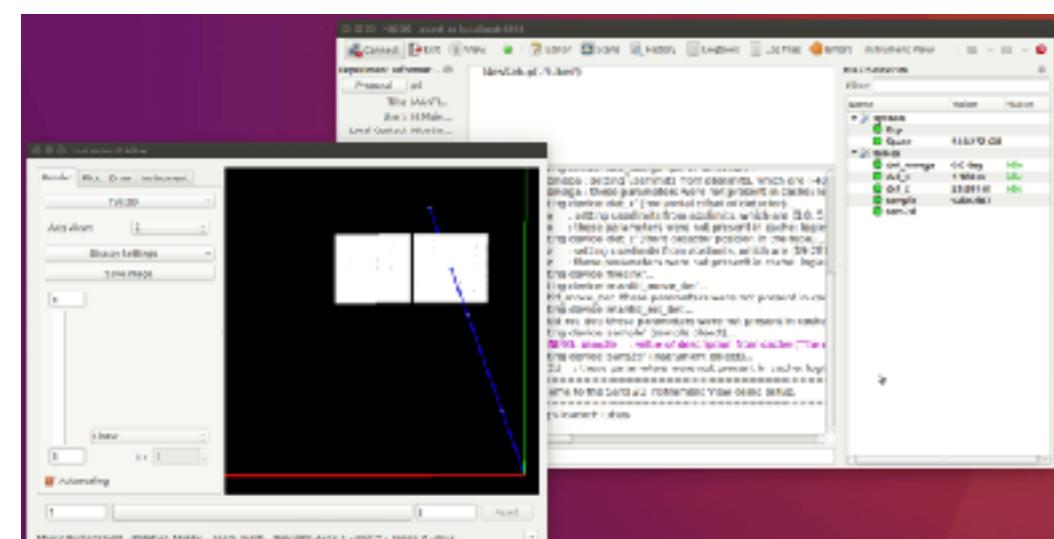
Imaging software centre QIM. Objective Focusing in on a Scandinavian Imaging centre

- ESS will join existing collaboration with DTU & MAXIV (DTU Lead)
- Ensuring Alignment of technologies and development at an early stage



Next generation data acquisition

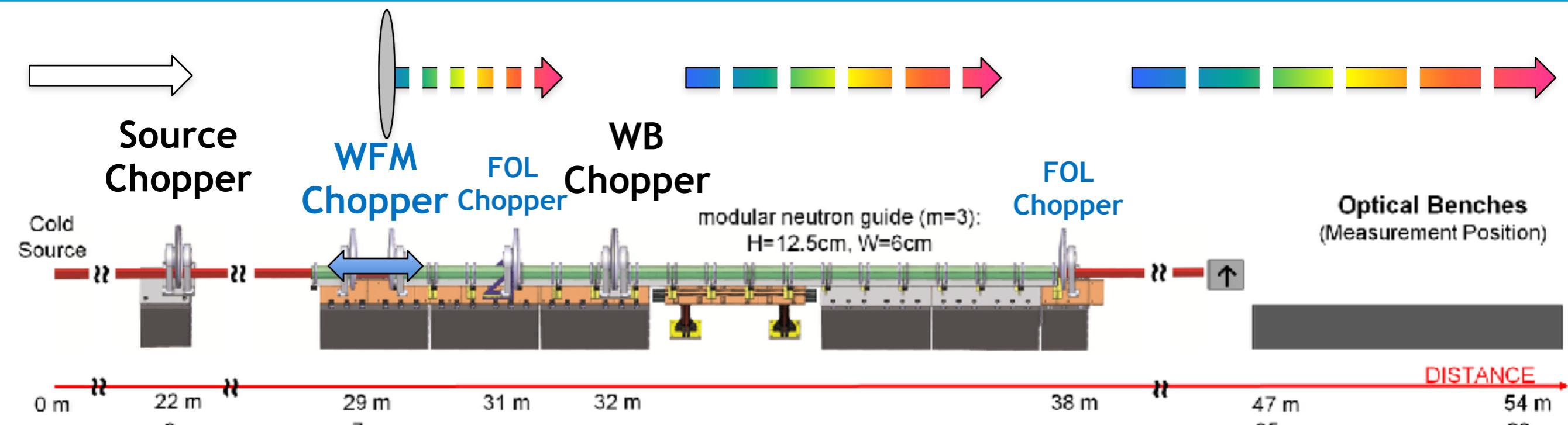
- Event mode data collection
- Fast capture of experimental metadata
- Big data technology
- FAIR data from the start
- High performance infrastructure, software data storage & data management
- Remote access to infrastructure



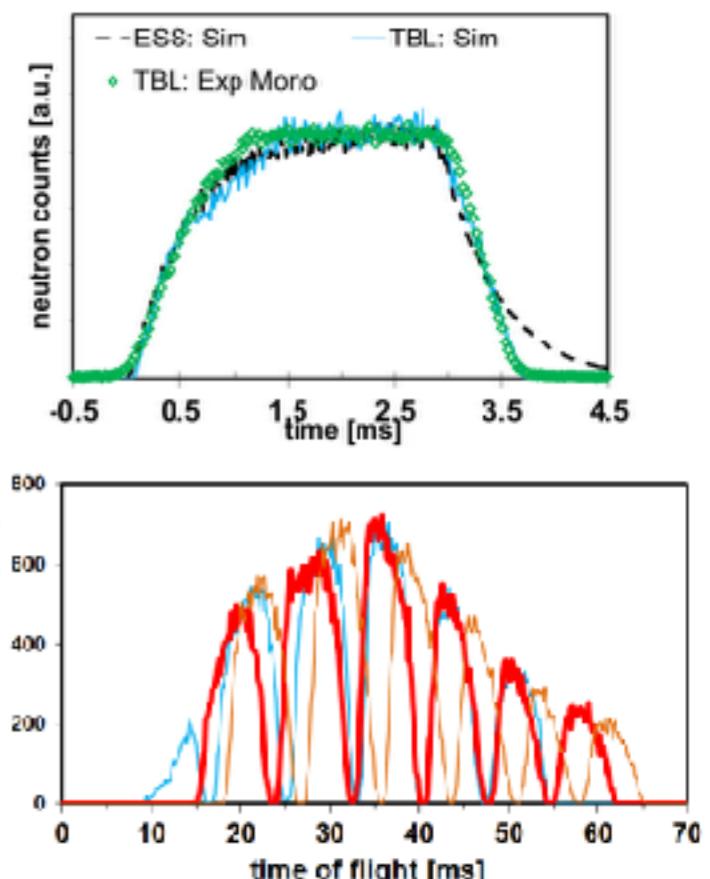
ESSIIP on V20 Test beam line



EUROPEAN
SPALLATION
SOURCE



- Deploy ESS controls & DAQ stack
- Full scale prototype tested 22-25 /1/18
- Tests controls and DAQ architecture
- Prototypes WFM mode data processing



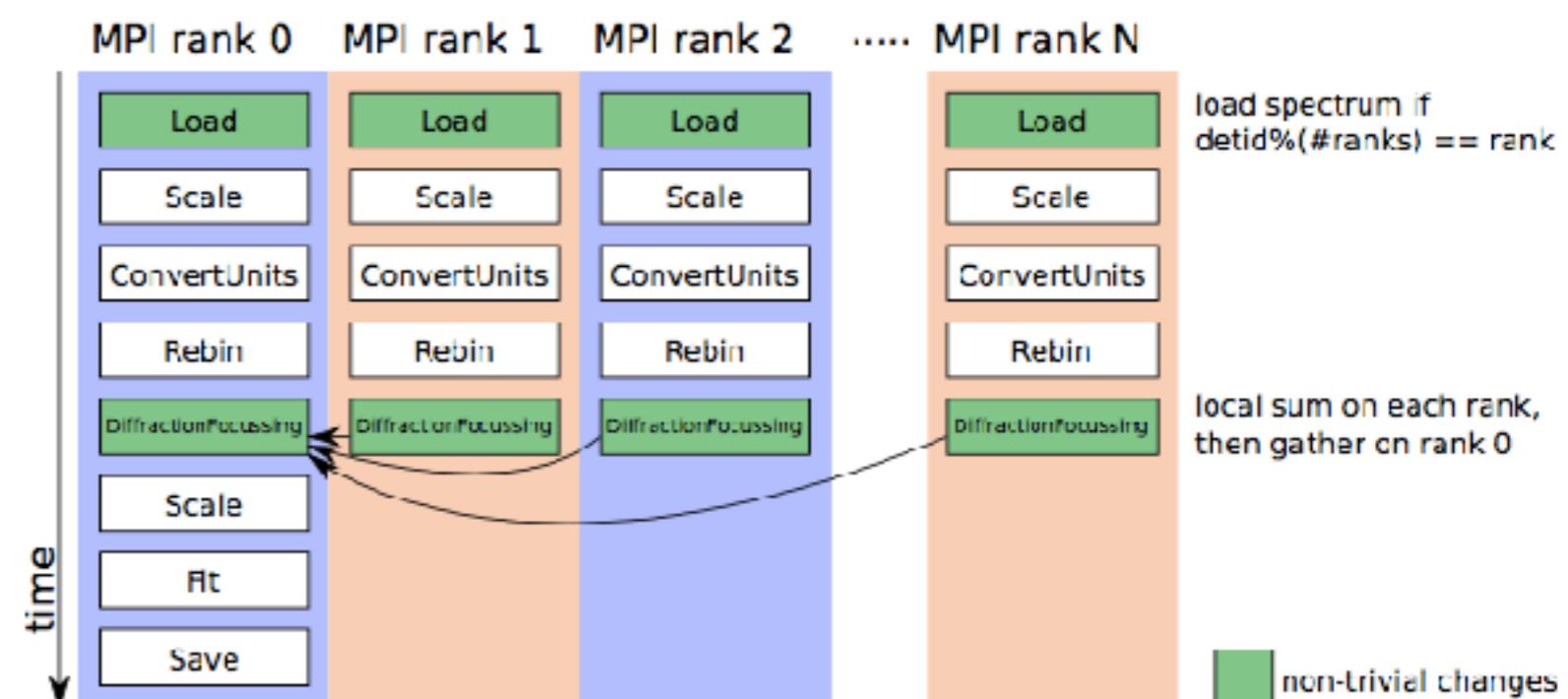
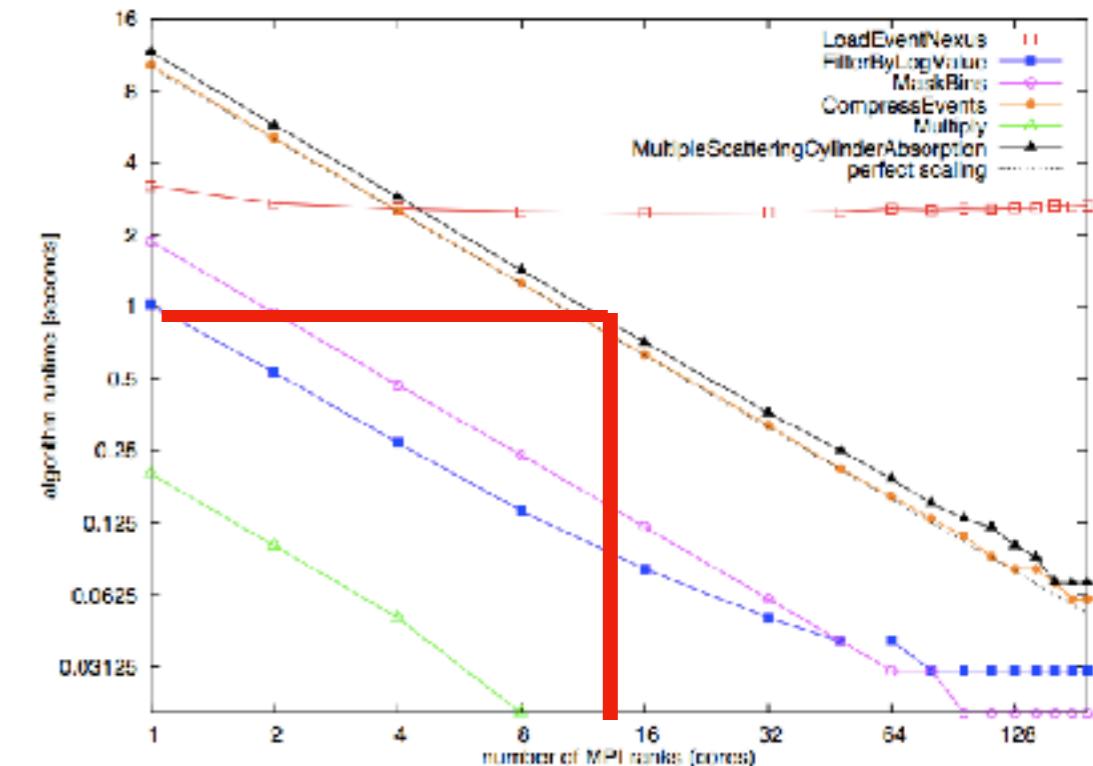
Make FAIR data processing Fast



- ▶ Histogram data type
- ▶ Instrument geometry
- ▶ MPI processing
- ▶ MPI data loading
- ▶ Prototype MPI MD event WS
- ▶ Core team proposal



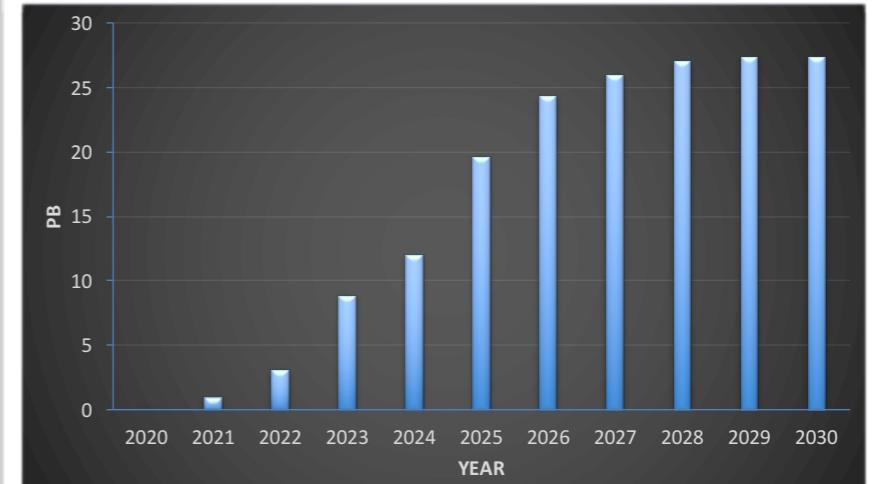
ISIS



Data Management



- ▶ ESS will produce a lot of data
- ▶ 8GB / Minute / Instrument



- How do I get it
- How do I look at it
- What does it mean

SciCat A new open source meta data catalogue



- Raw Data
- Meta Data
- Analysed Data
- Optimised for ESS
- Deployed at MAXIV & PSI



PAUL SCHERRER INSTITUT

A screenshot of the SciCat web interface. At the top, there is a navigation bar with tabs for 'SEARCH', 'DATA', 'SAMPLE DATA ENTRY', 'DATA', 'REGISTER', and 'HELP'. Below the navigation bar is a search bar with placeholder text 'Search...'. On the left, there is a sidebar with sections for 'EXPERIMENTS' (listing 'Results: 274'), 'Baseline' (with a dropdown menu), 'Group' (with a dropdown menu), and 'Date Range' (with a dropdown menu). The main area displays a table of search results. The columns are labeled: 'Correlation ID', 'Run ID', 'Creation Time', 'Group', 'Proposal ID', 'Analysis Status', and 'Delete Status'. The table contains multiple rows of data, each corresponding to a different experiment entry. The first few rows show entries such as '188/00224/0083 1/0411/2020/Monochromator_1_m_0002', '188/00224/0083 1/0412/2020/Monochromator_1_m_0002', and so on.

European Open Science cloud



Pan European FAIR Data

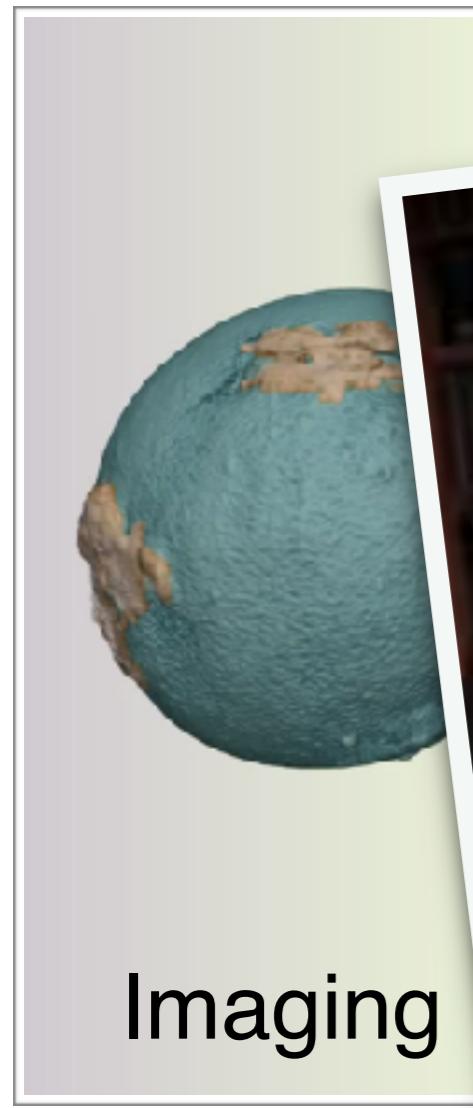
- My data are your data...
- Photon and Neutron Open Science Cloud
 - Data Federation
 - Open Services for data treatment and analysis
 - Access to compute services



Complexity defines the ESS science case



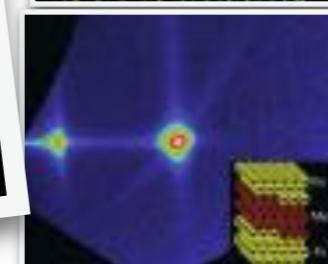
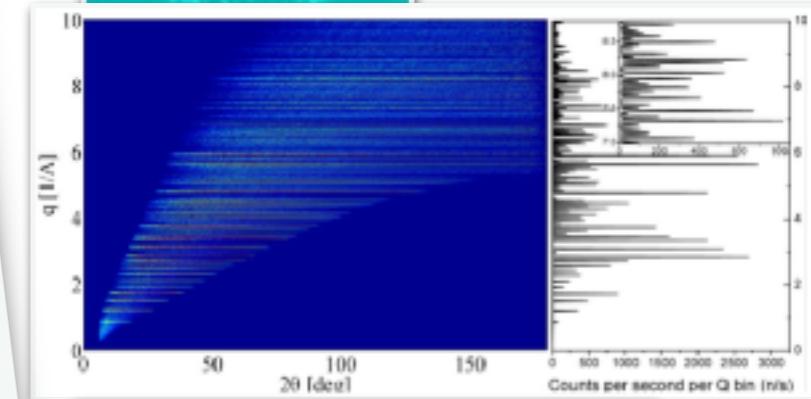
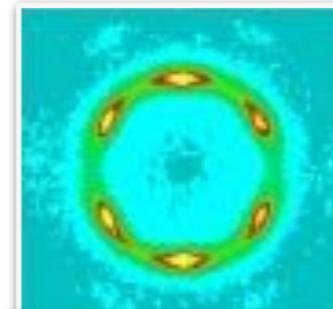
EUROPEAN
SPALLATION
SOURCE



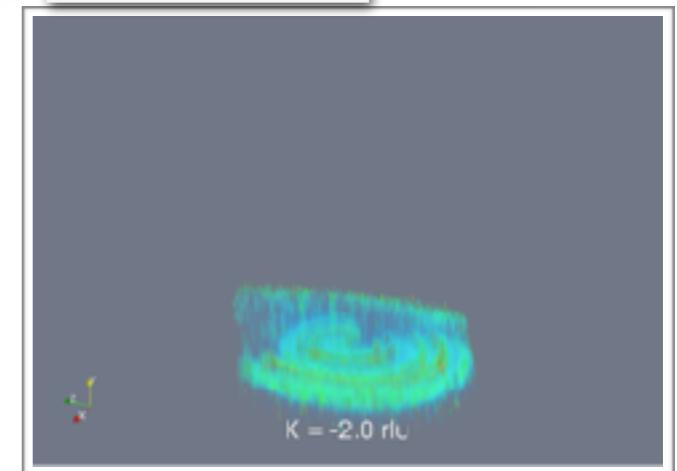
Imaging



SANS



Spectroscopy



Inelastic Neutron Scattering



ESS - PSI - ISIS Collaboration

Part of the ISIS PACE project

"Rietveld for inelastic" required for over 60% of experiments

High performance generation of 4D datasets

High performance Spin wave modelling and resolution convolution

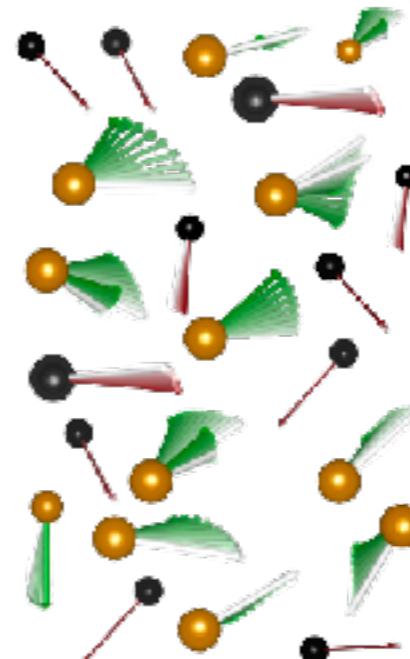
Multiple solvers & models

Linear spin wave, Dimer, coupled dimer

Atomistic spin dynamics

Refactor and modularise SpinW

Add other 'solvers' to the UI layer



ILL / ESS collaboration on Fullprof



ILL and ESS has agreed to collaborate on curating and modernizing Fullprof

What we want to achieve

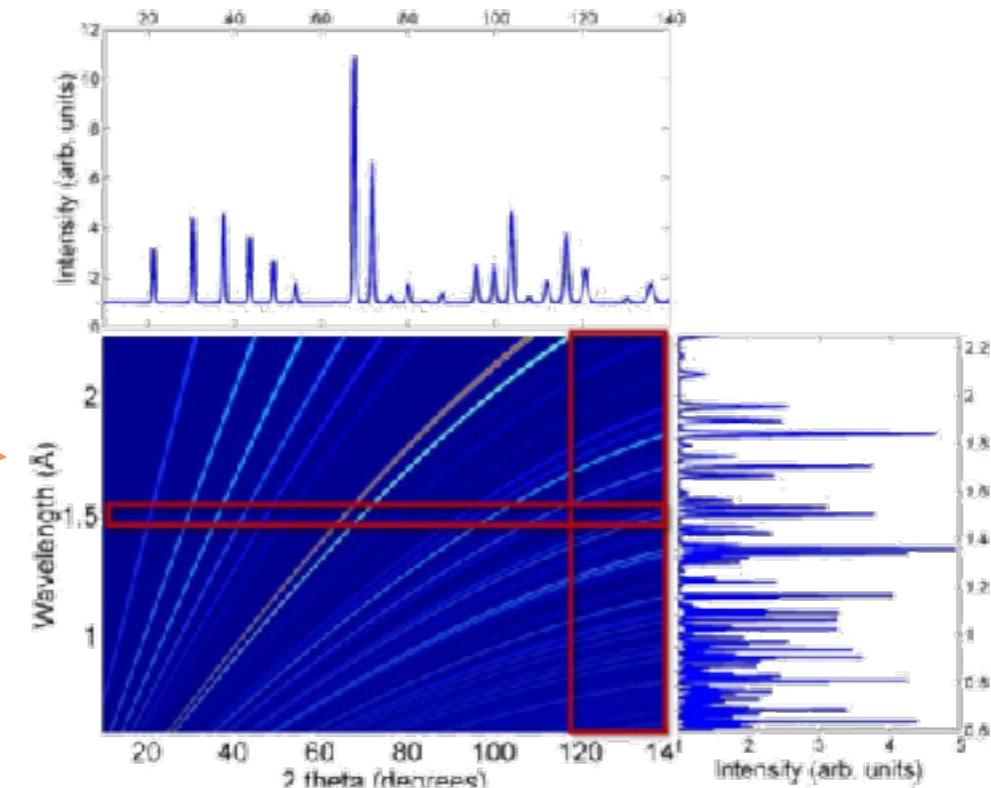
- ✓ Python scripting interface
- ✓ User-friendly GUI
- ✓ Documentation
- ✓ Modern software dev. env.
- ✓ 2D Rietveld
- ✓ Open source
- ✓ No single point of failure



Jenkins



Juan Rodriguez-Carvajal



(Mogens Christensen)

DFT calculations and cluster expansion

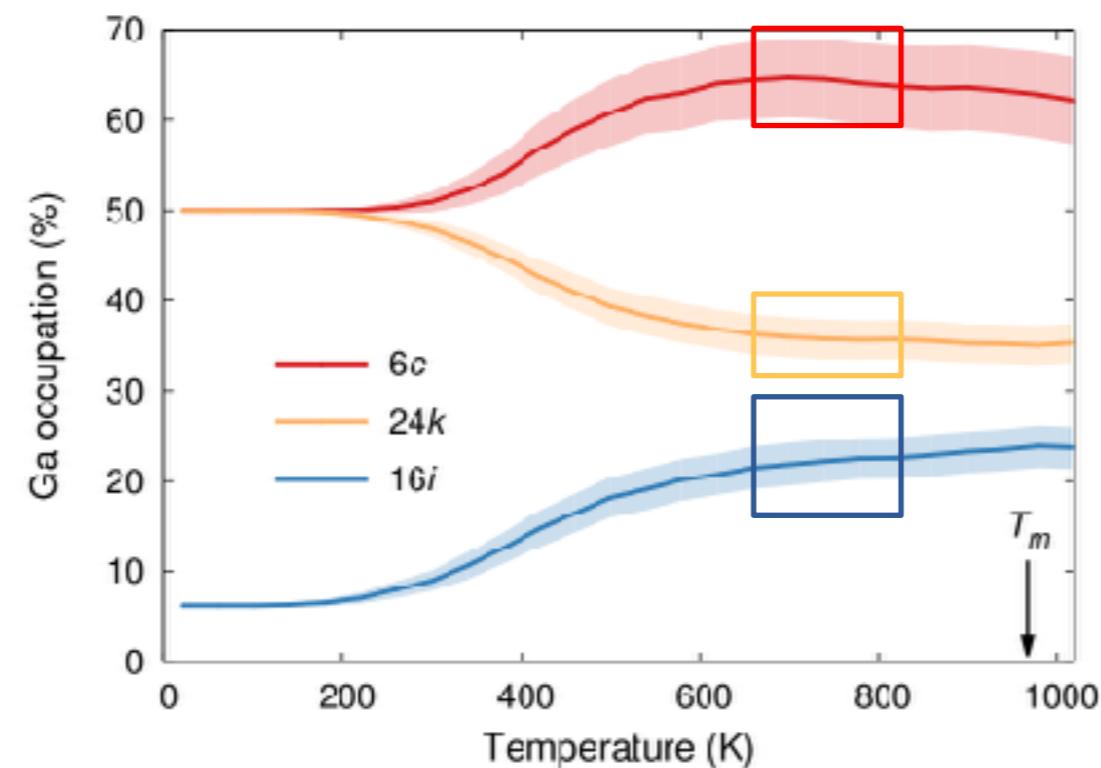
Goals:

Make IceT/MCHammer

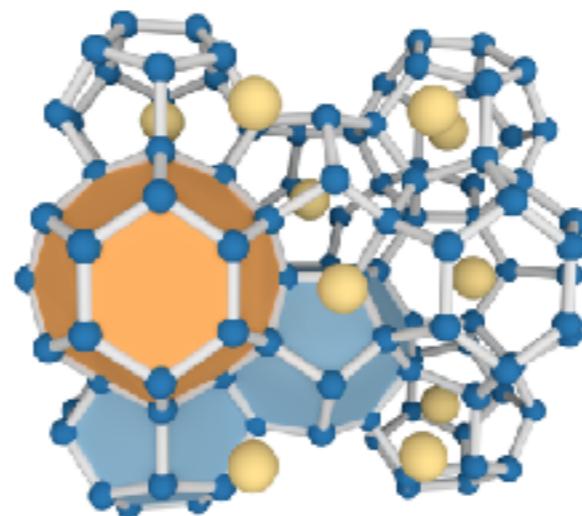
1. Sustainable software
2. Available for ESS users



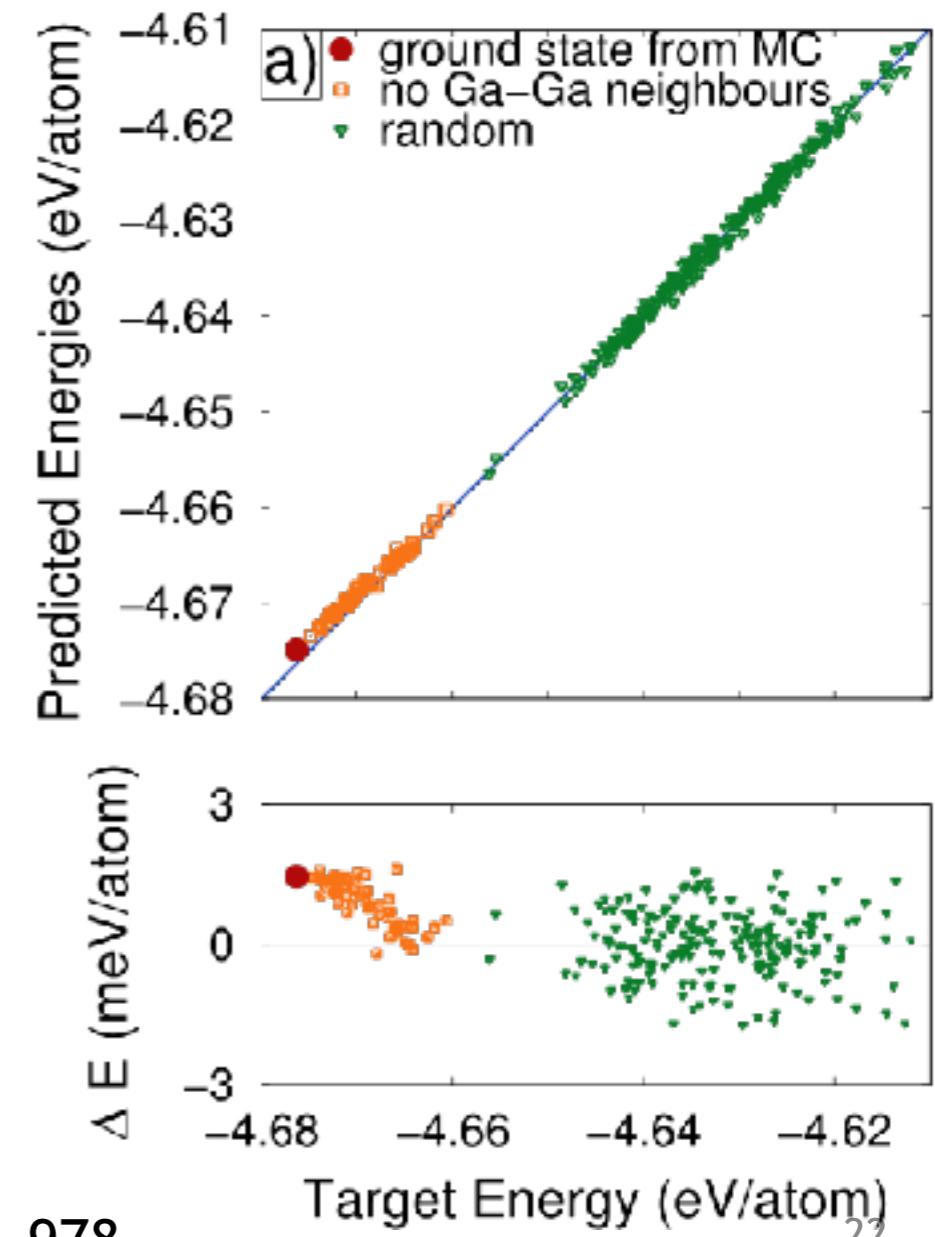
CHALMERS



Exp.: Christensen *et al.*, Dalton Trans. 39, 978
(2010)



Ångqvist & Erhart, Chem. Mat.



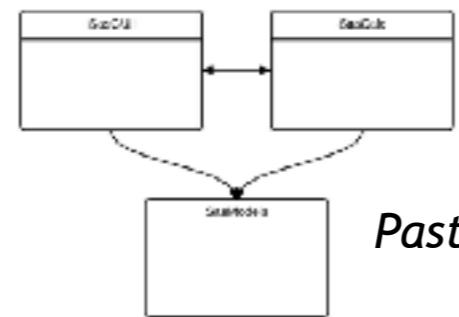
SasView



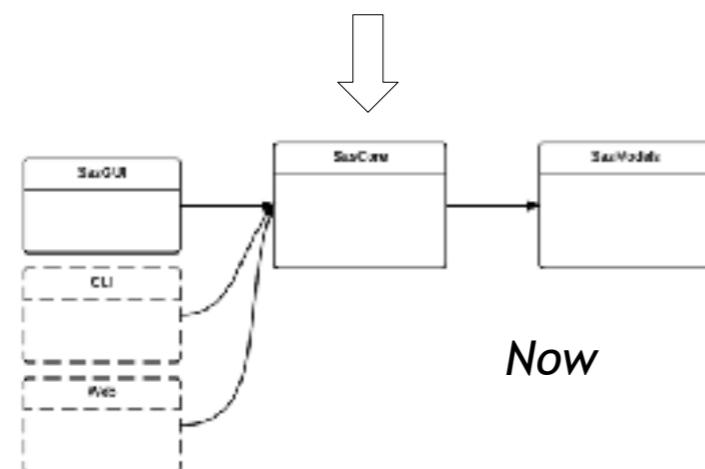
SasView code camp @ TUD

ESS is important partner in SasView dev. community

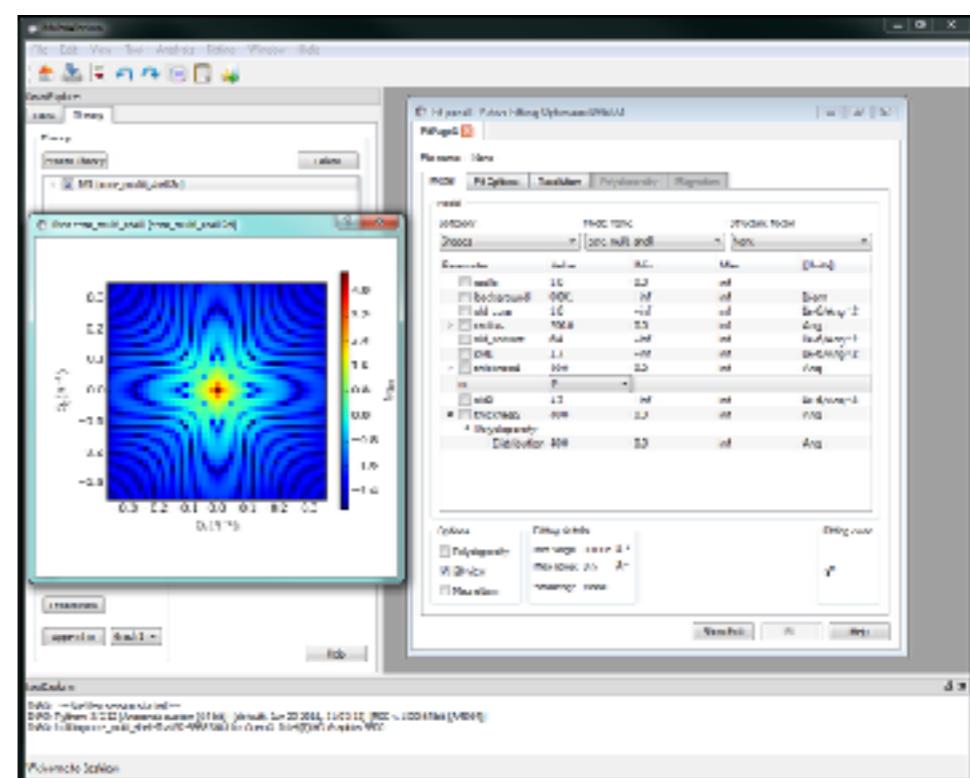
- Aligned ESS and SasView roadmaps
- Proper development processes using
- Hosting build services for community.
- Refactored / modularized SasView
- Enabling SasView models to be used in McStas
- Integrating SasFit models - some license issues
- Developing new GUI and CLI (Python API) for V5



Past



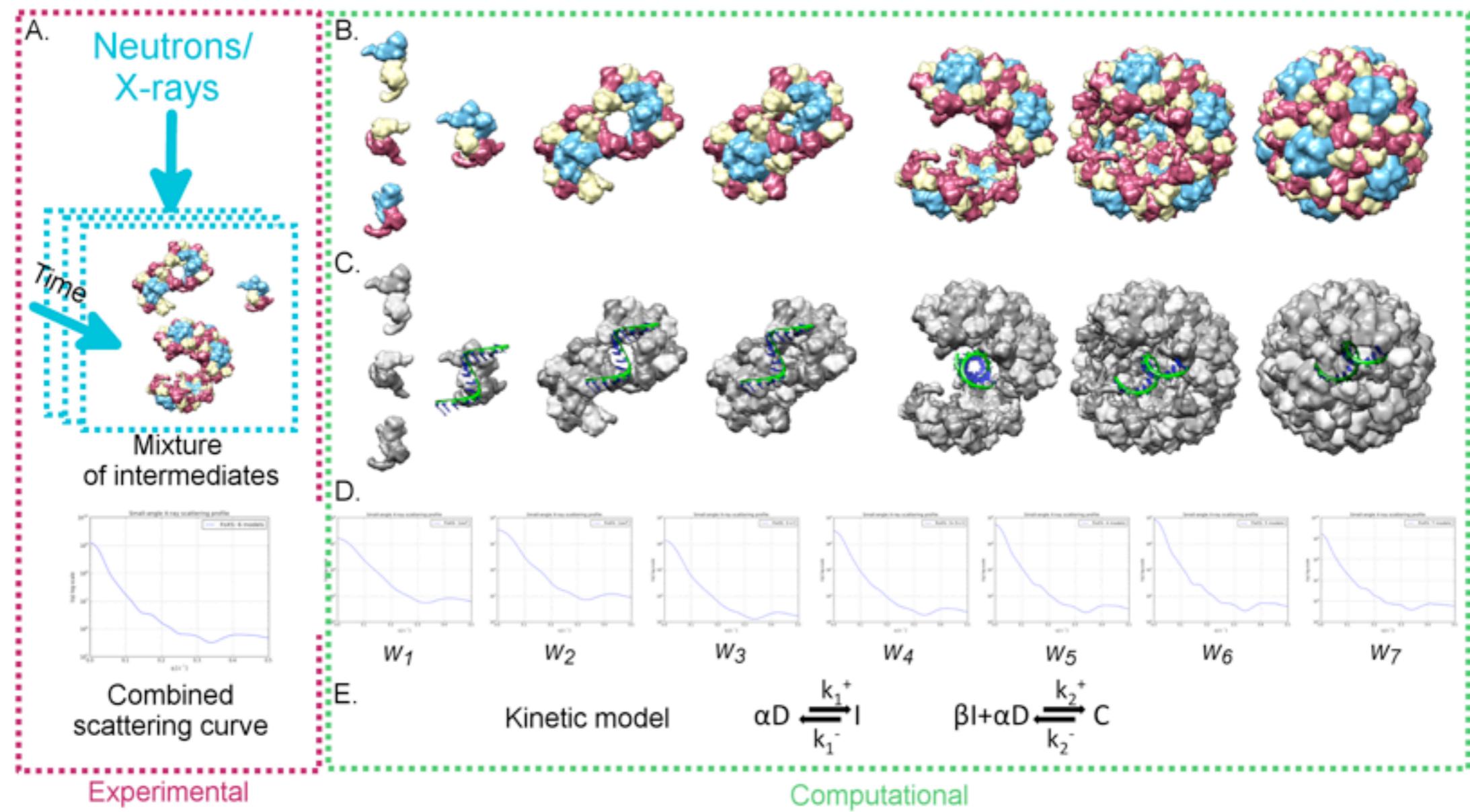
Now



Protein self-assembly studied with time-resolved SANS/SAXS



Vetenskapsrådet



Fitting potentials to QENS data (dynamical version of the EPSR method)

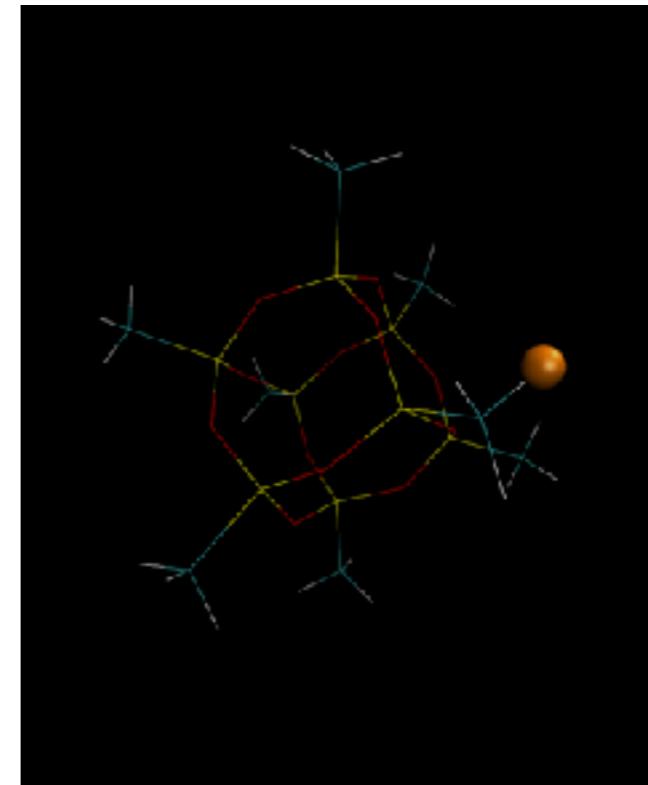
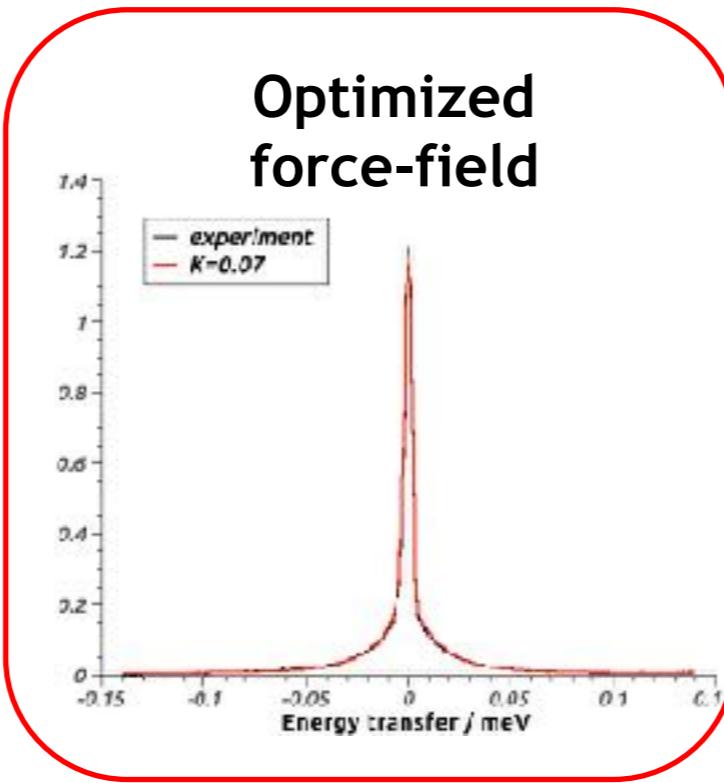
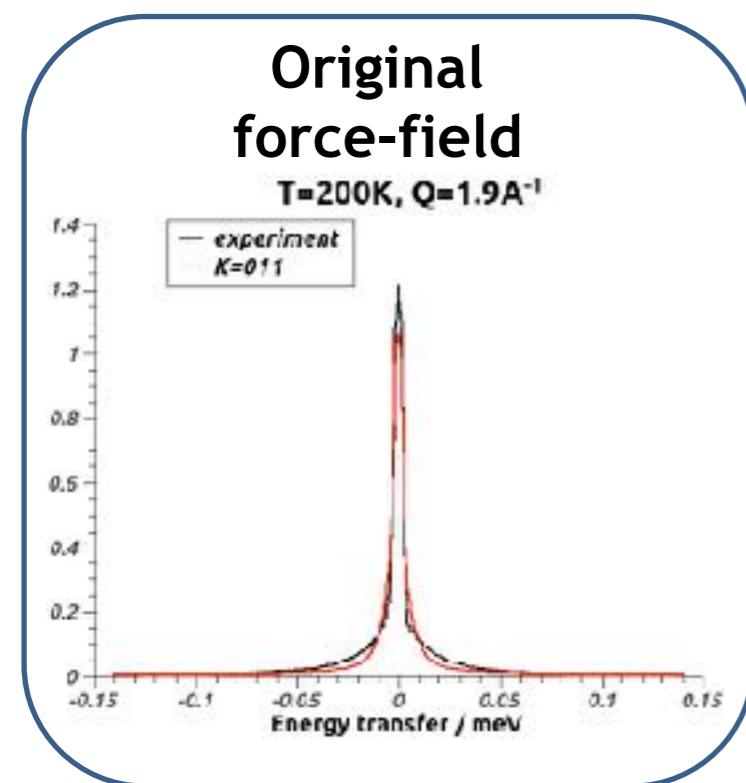


Science & Technology Facilities Council
ISIS



Vetenskapsrådet

Methyl rotations in methyl-Polyhedral oligomeric silsesquioxanes



Mark Hagen, Jose Borreguero (SNS/NDAV), Mike Crawford (Dupont), Niina Jalarvo (Julich)

Any questions?



<https://europeanspallationsource.se/careers/vacancies>