

Modelling & Simulation session

16:00 -> 17:40

16:00	Thomas H. Rod, ESS	Computing for materials science at the European Spallation Source ERIC
16:20	Martin Morhac, SOVIA Digital	Industry 4.0 - Slovakia reality
16:40	Otto Petraska, BSH	Effectivity of the application of experimental and simulation methods in the development of NVH measuring stations in industrial production
17:00	Ludek Zalud, CEITEC, Brno University of Technology	Demonstration Testbed for Industry 4.0 at Brno University of Technology
17:20	Erik Prada, ZTS VVU, Cluster AT+R	Modelling of nonholonomic multibody robotic systems using geoemtric mechanics methods

Computing for materials science at the European Spallation Source ERIC

Thomas Holm Rod

Group Leader Data Analysis and Modelling, ESS

**Academia-Industry Matching Event on the Mutual Impact of Industry 4.0
and High-Energy Physics,
15-16 March 2018, Grand Hotel Stary Smokovec**

www.europeanspallationsource.se

15 March, 2018

- Overview of European Spallation Source ERIC
- Some use cases
- Integrated and automated data processing
- Challenges related to providing scientific efficiency

ESS will be the brightest neutron source

Proton Accelerator (Linac)

- 2GeV, 50mA, 5MW on target
- Frequency: 14Hz

Neutron Beam Instruments

- 16 Instruments in construction budget

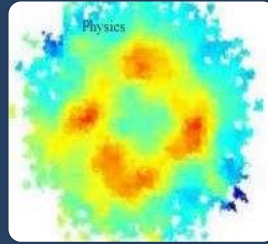
Target & Moderators

- Rotating wheel of W
- Frequency: $\sim 0.4\text{Hz}$
- High brilliance LH moderators



Material science - broad time and length scales

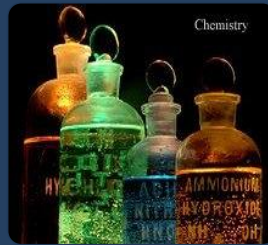
PHYSICS



ANGSTROMS AND PICOSECONDS

- electronic and magnetic structure
- strongly correlated electron systems

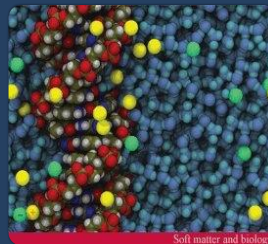
CHEMISTRY



NANOMETRES AND NANOSECONDS

- chemical structure and dynamics
- structure/property relationships

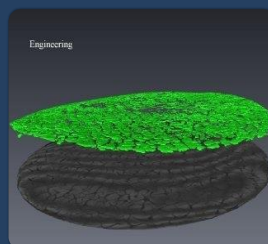
SOFT MATTER & BIOLOGY



MICRONS AND MICROSECONDS

- interfaces, micelles, etc.
- protein structure and dynamics

ENGINEERING & MATERIALS SCIENCE



METRES AND MONTHS

- engineering measurements, heritage science
- tomography, residual stress, etc.

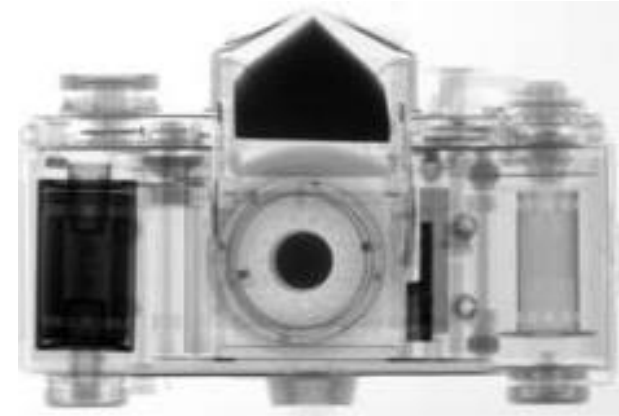
Neutrons see hydrogen through metal



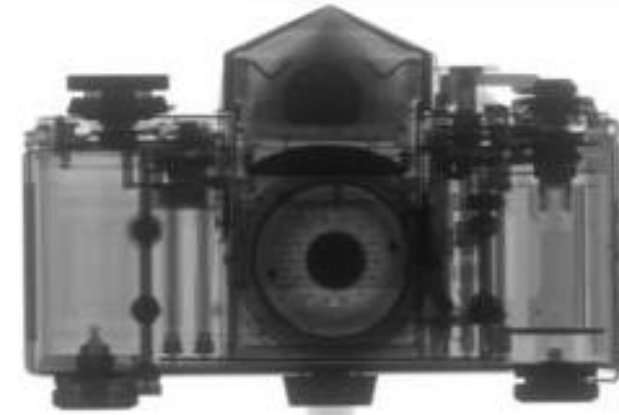
Anders Kaestner



<https://youtu.be/VESMU7JfVHU>



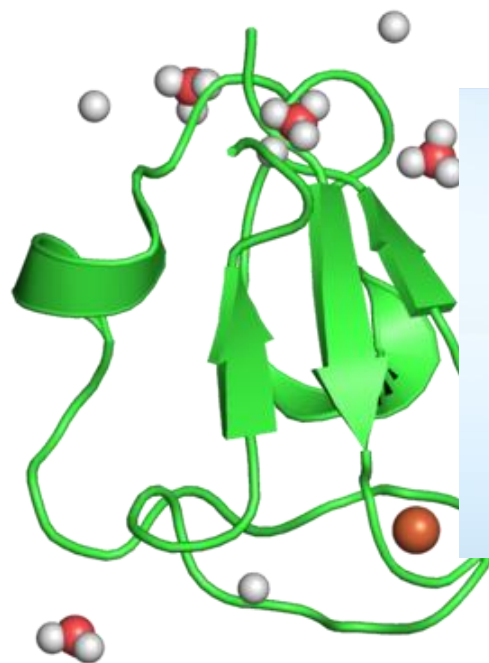
Neutrons



X-rays

We can see protons in crystal structures

Rubredoxin



Cuypers et al., Angew. Chem.
Int. Ed. Engl. (2012)
PDB ID: 4ar3

H-FABP



Podjarny et al., IUCrJ (2016)
PDB ID:5ce4

Current situation

February 2018

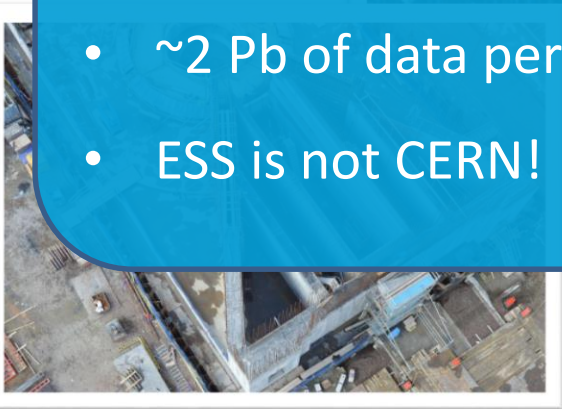


Start of user programme 2023

Steel & concrete – it's happening



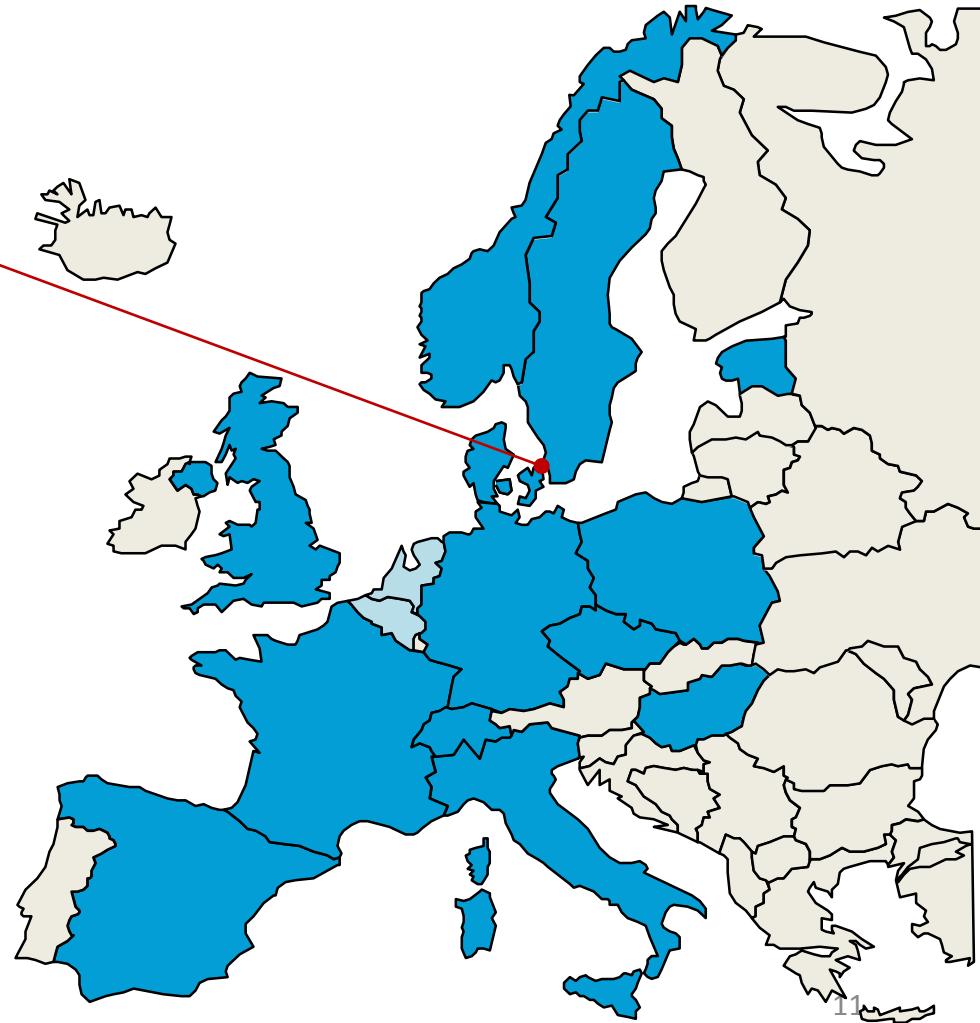
- 1.843 billion Euro construction project
- ESS is (primarily) for materials science
- 2-3000 visiting scientists per year
- ~2 Pb of data per year
- ESS is not CERN!



ESS is a Pan-European collaboration

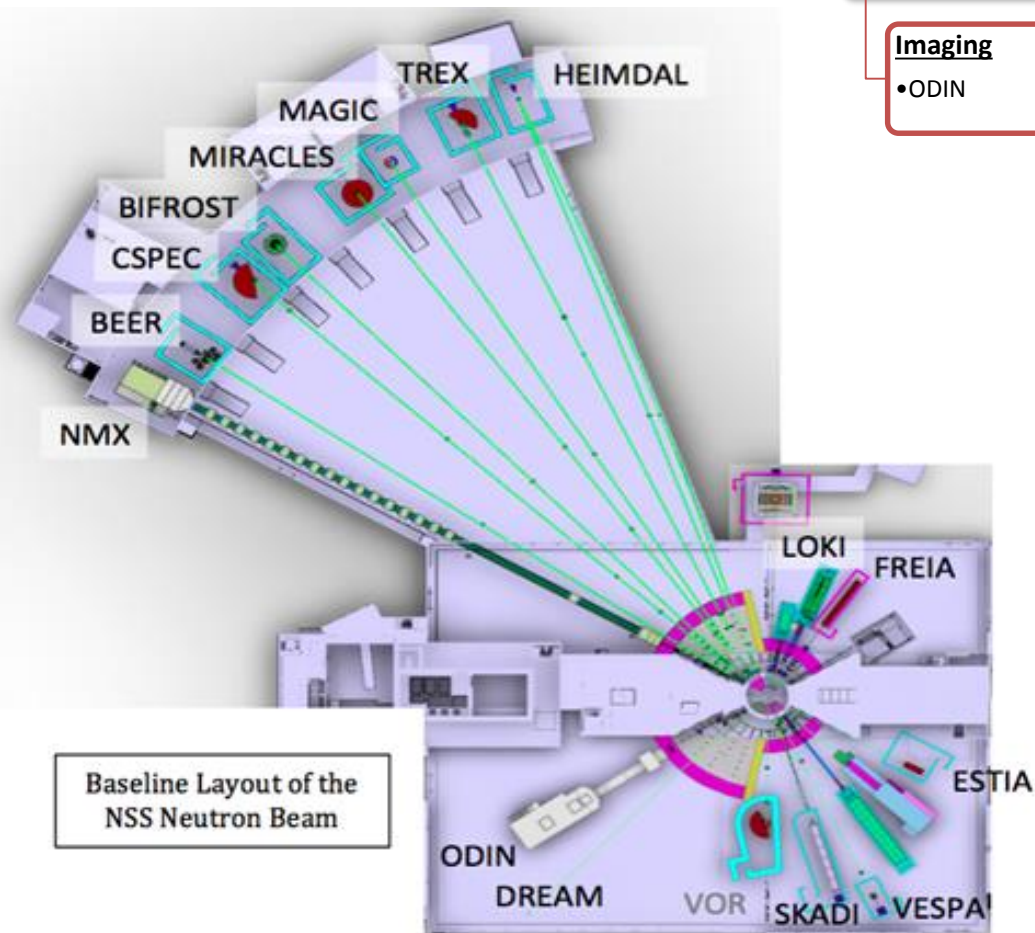


- Sweden & Denmark are host nations
- 15 member countries
- +100 laboratories contribute
- User program starts 2023
- 15 instruments planned
- 2-3000 visiting scientists per year



The ESS tool kit & user program

Instrument feature series at esss.se



Imaging

Imaging

- ODIN

Diffraction

Engineering

- BEER

Powder

- DREAM
- HEIMDAL

Single Cryst.

- MAGIC

Macromol.

- NMX

Large-scale structures

SANS

- LoKI
- SKADI

Reflectom.

- ESTIA
- FREIA

Spectroscopy

Molecular

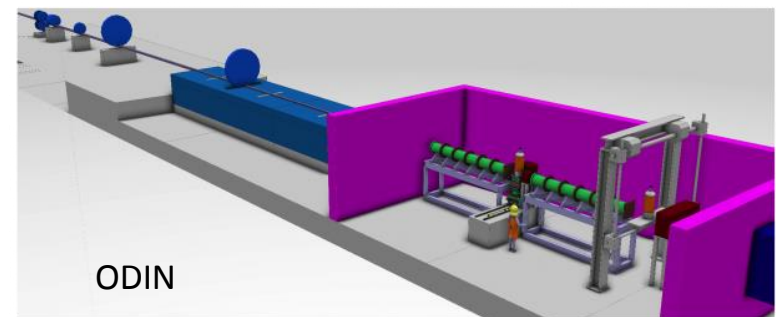
- VESPA

QENS

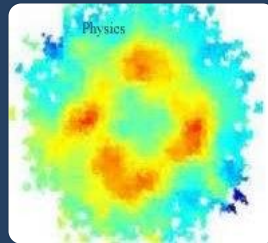
- C-SPEC
- MIRACLES

INS (Sxtal)

- BIFROST
- T-REX



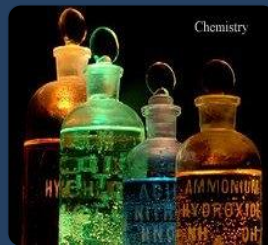
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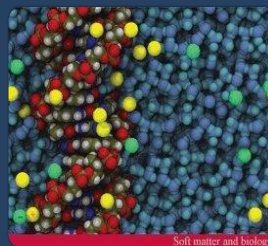
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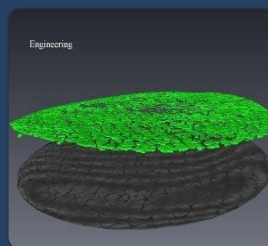
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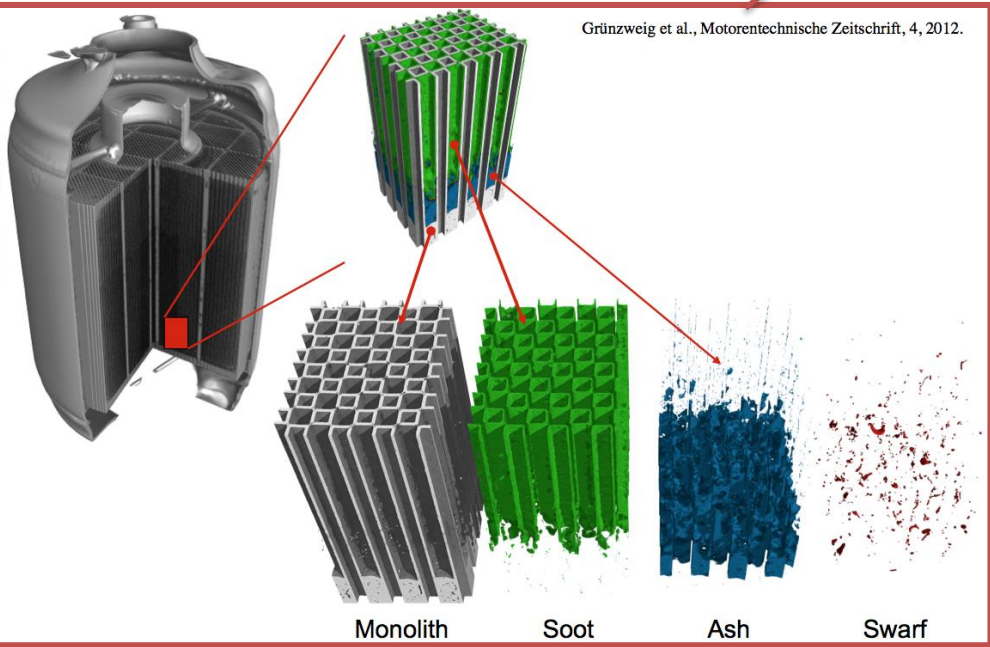
- engineering measurements, heritage science
- tomography, residual stress, etc.

The ESS Tool Kit - Imaging

Grünzweig et al.,
Motortechnische Zeitschrift (2012)

Imaging
•ODIN

Grünzweig et al., Motortechnische Zeitschrift, 4, 2012.



Diffraction

Engineering

- BEER

Powder

- DREAM
- HEIMDAL

Single Cryst.

- MAGIC

Macromol.

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Large-scale structures

SANS

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Reflectom.

- ESTIA

Spectroscopy

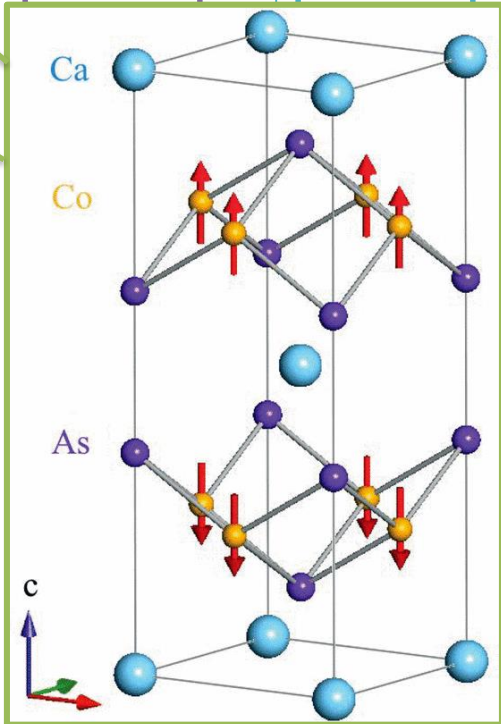
Molecular

- VESPA

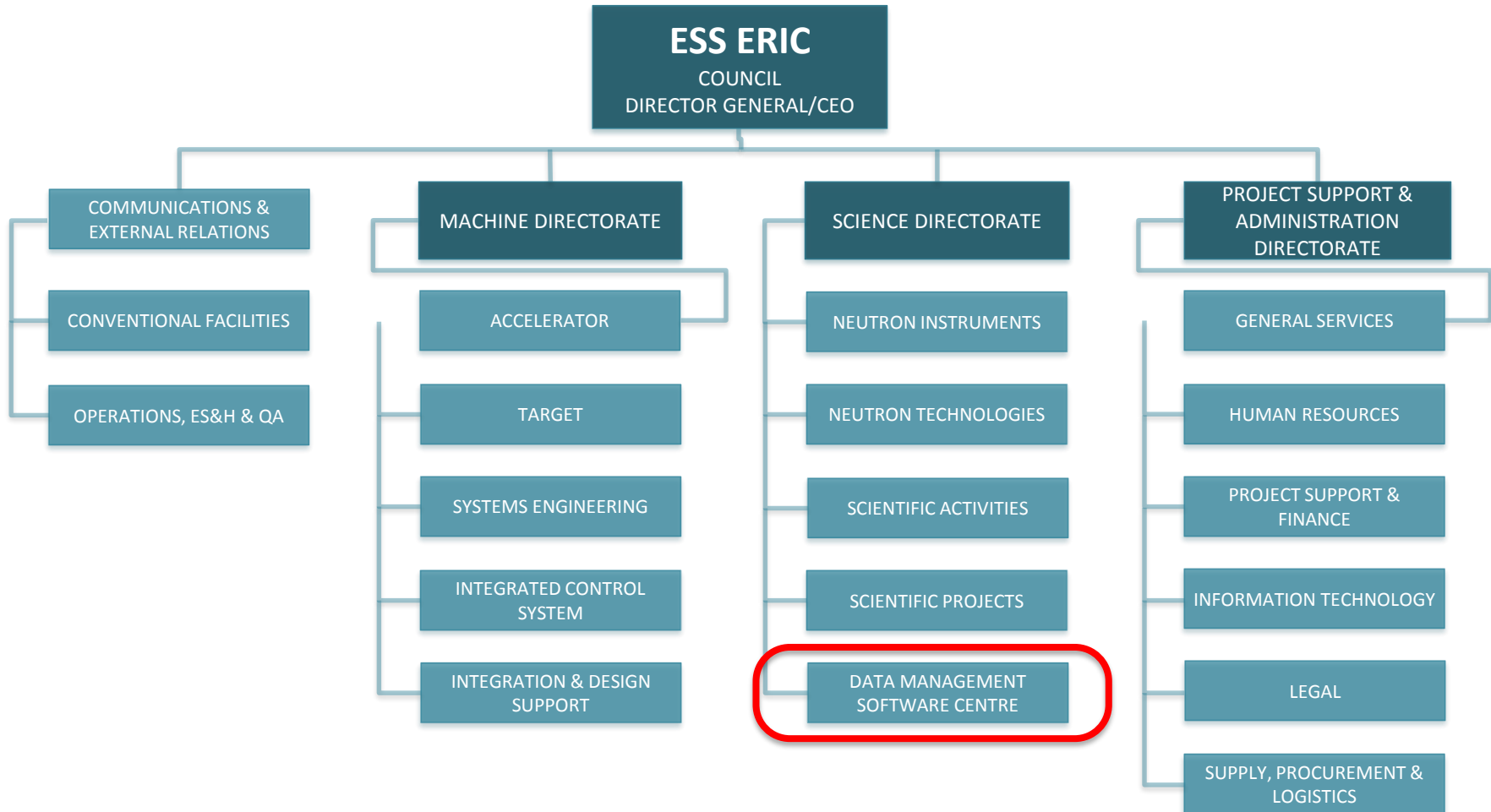
QENS

- C-SPEC

CaCo_{1.86}
Quirinale,
Phys. Rev. B (2013)



DMSC - Scientific computing for ESS



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.

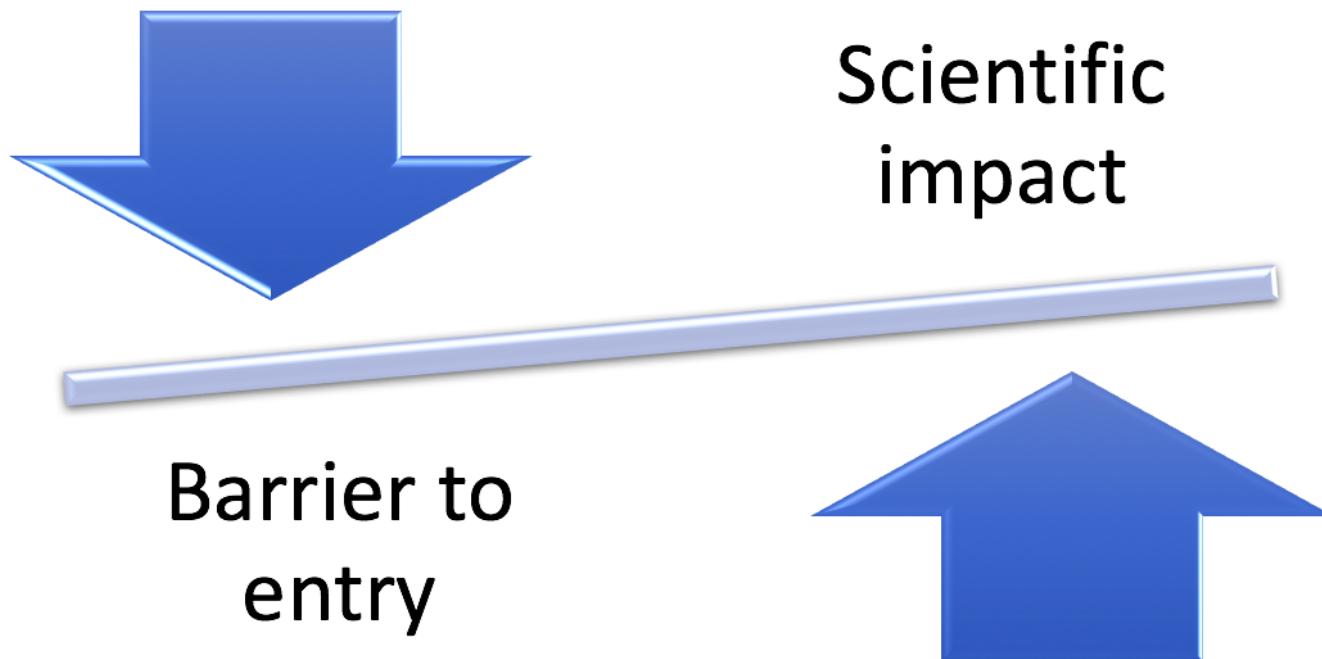
- Dual location - Lund & Copenhagen
- Data management and curation

User programme support

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

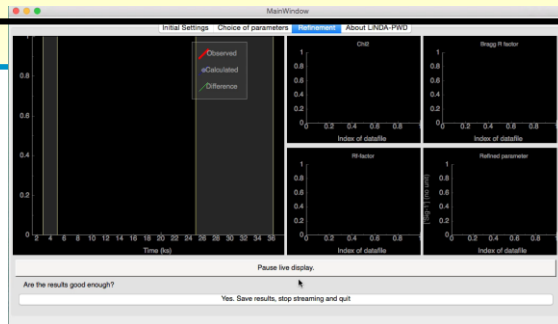
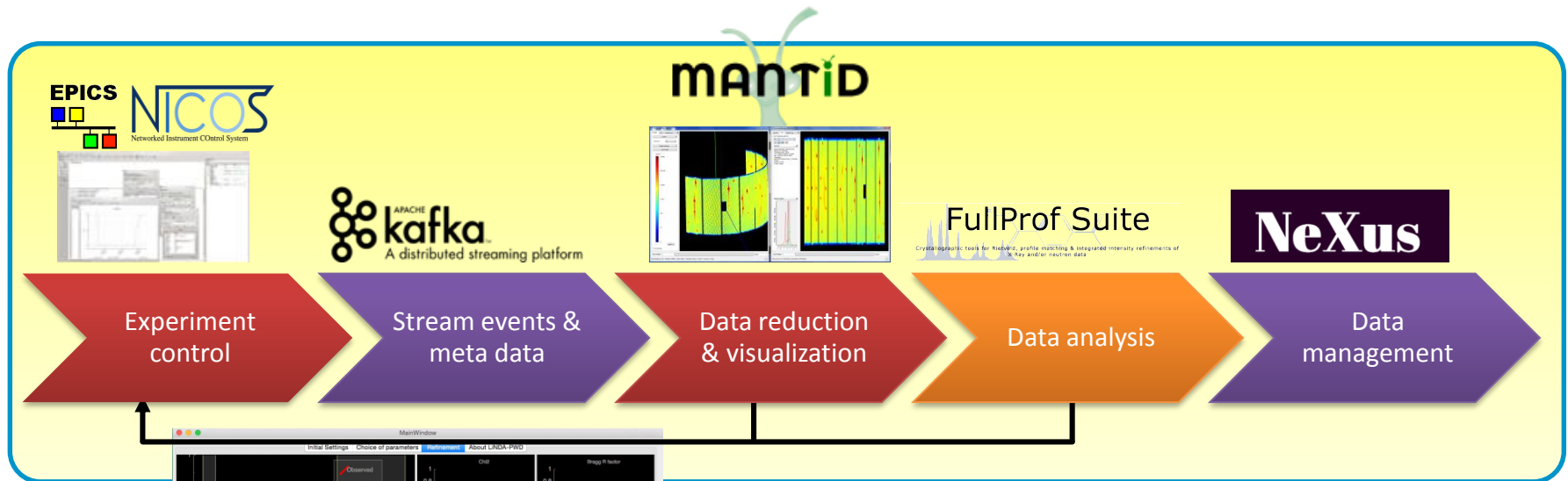


- Minimise the time it takes to understand experimental data



- Maximise the scientific impact and scientific success of ESS

Integrated data processing pipeline



Preferred languages

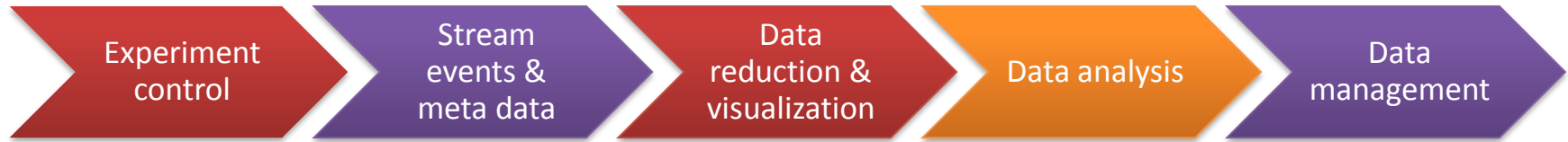


Some initiatives

- Make *integrated* data processing pipeline work smoothly, seamlessly, and *real-time*
- For each step provision *sustainable* software
- Need *automation* for smooth and efficient workflow and good user experience

Testing event streaming without instruments

- We want to test data processing pipeline on virtual data

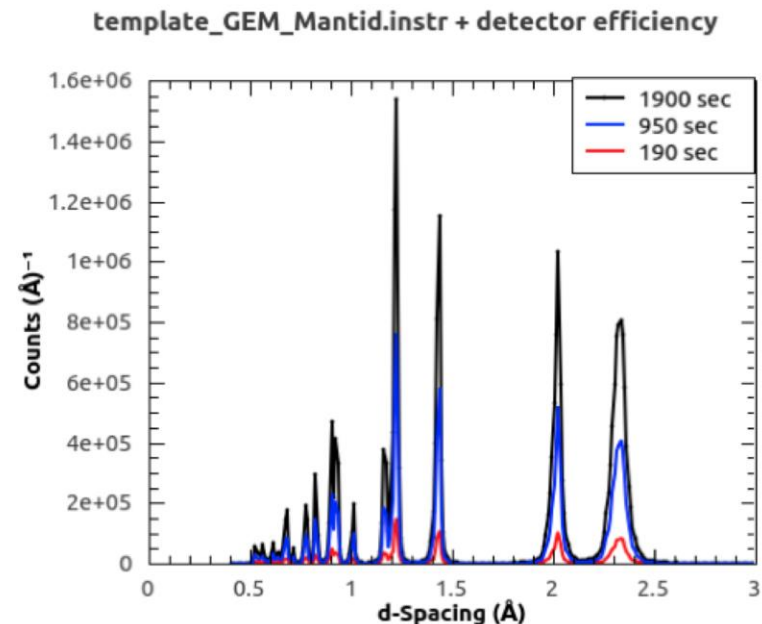


We can generate virtual data stream

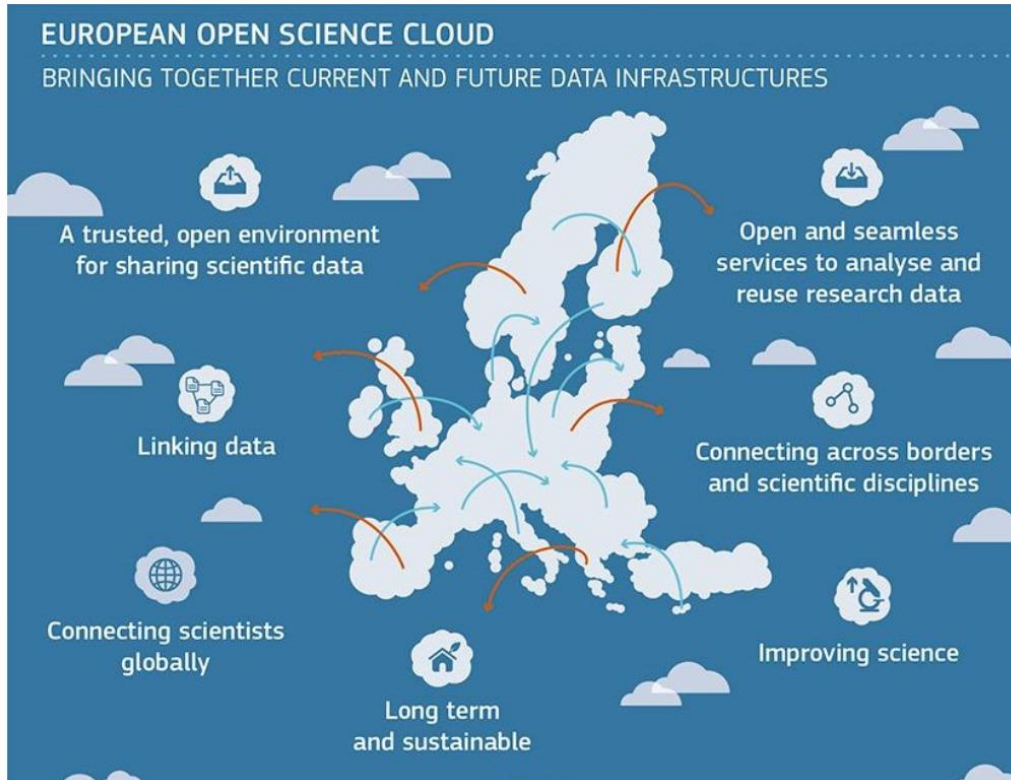
useful

for

- testing
- experiment planning
- teaching



European Open Science Cloud (EOSC)



Open access to FAIR data and associated (analysis) services through a one-stop shop

- F: Findable
- A: Accessible
- I: Interoperable
- R: Reusable



Consortium of P&N Sources:



Scientific efficiency need software – also for analysis, modelling and simulations

Challenges

Many different and independently developed software packages are needed

- Technical debt
- Single-point of failure
- Lack of standards
- Poor documentation – if any
- Closed software
- *Not* user-friendly
- Is not inter-operable
- Users are diverse

ESS will support ~15 programs for analysis



Methods:

- Fitting to models, specific for each technique and science
- Molecular dynamics simulations
Spin dynamics simulations
- Quantum chemistry methods
- Tomography incl. for ToF
- Monte Carlo simulations
- Machine learning methods

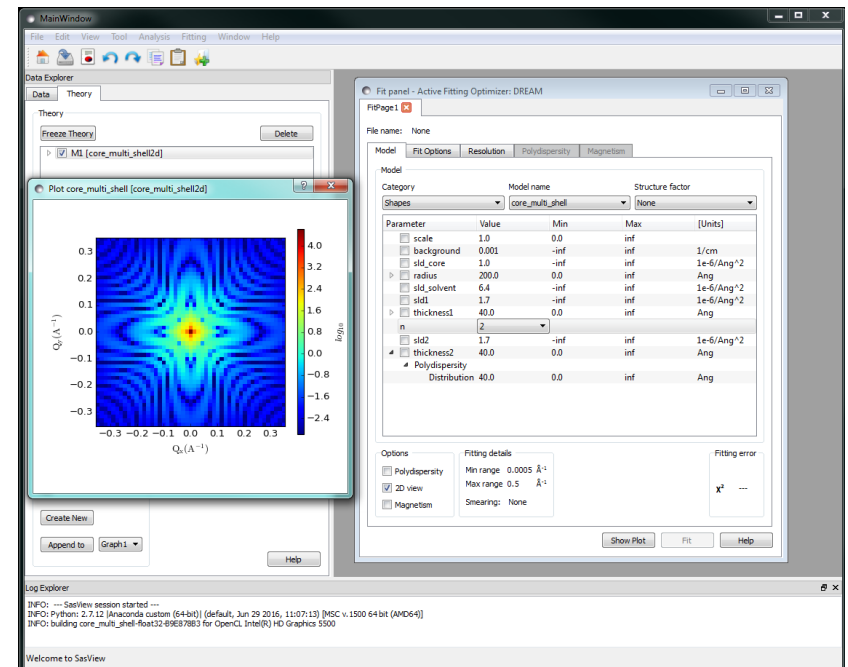
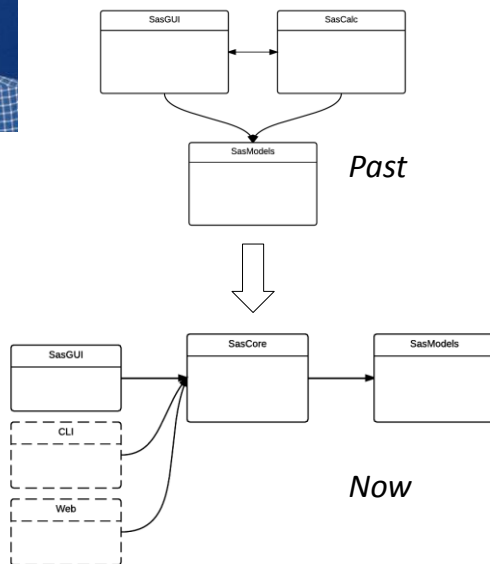
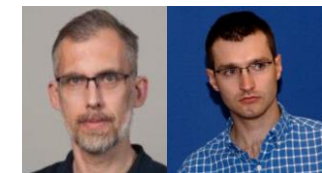




SasView code camp @ TUD

ESS is important partner in SasView dev. community

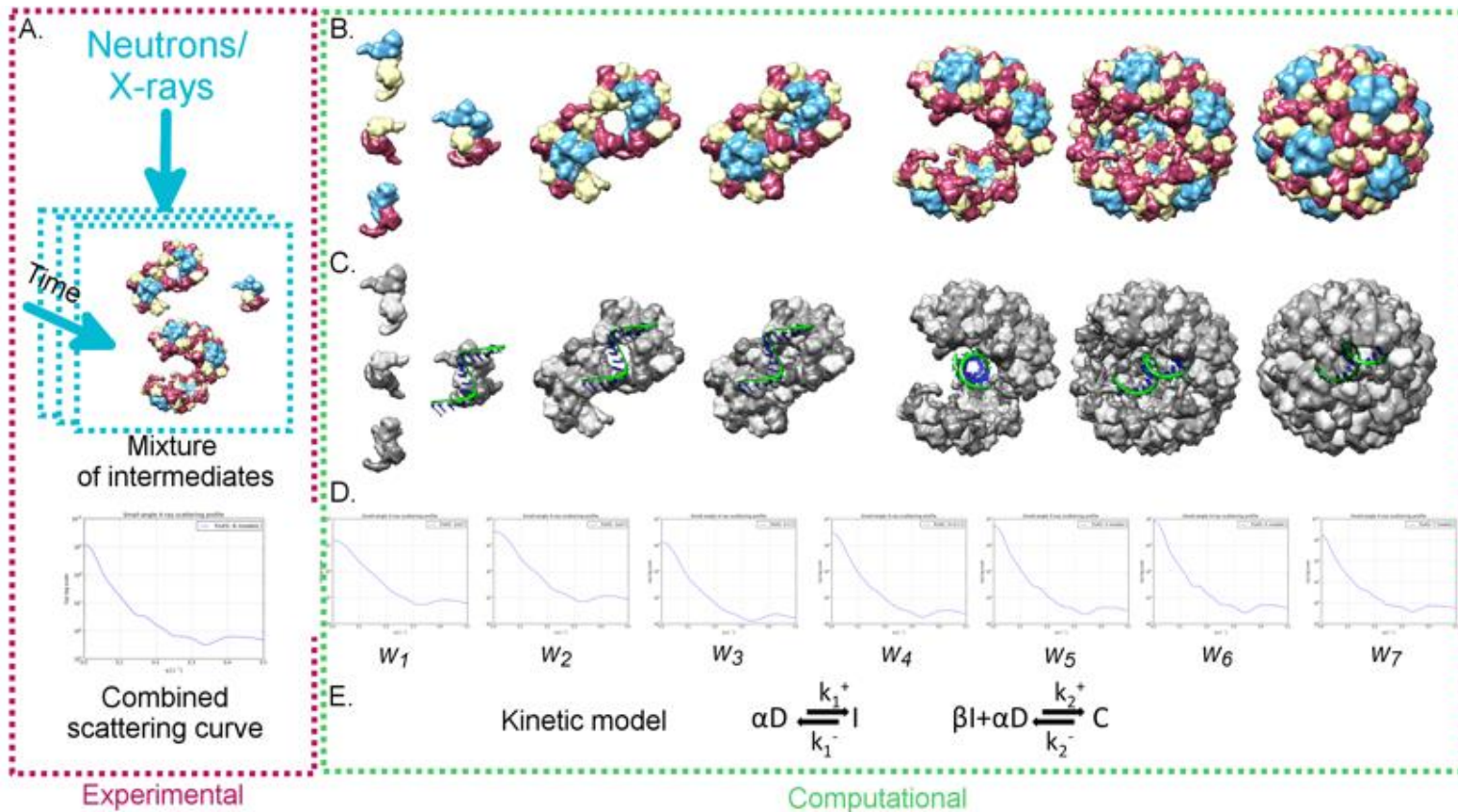
- Aligned ESS and SasView roadmaps
- Proper development processes using
- Hosting build services for community.
- Refactored / modularized SasView
- Enabling SasView models to be used in McStas
- Integrating SasFit models – some license issues
- Developing new GUI and CLI (Python API) for V5



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

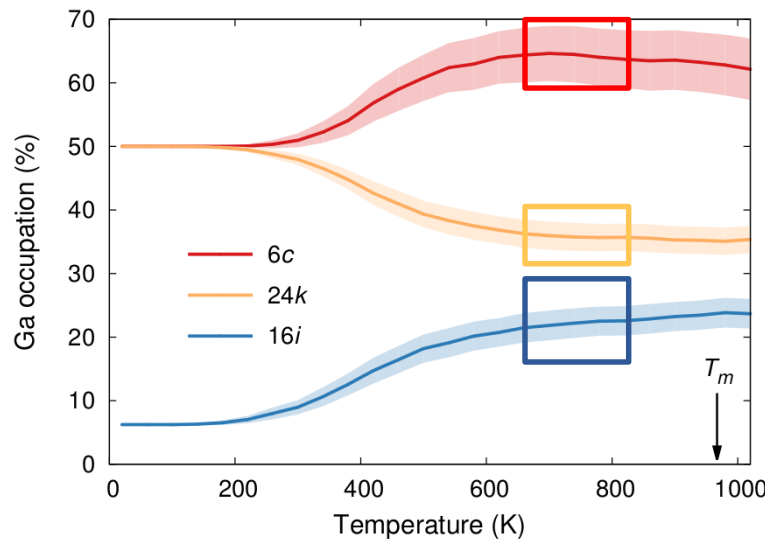
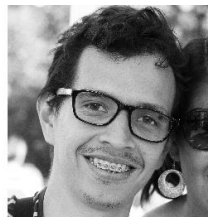
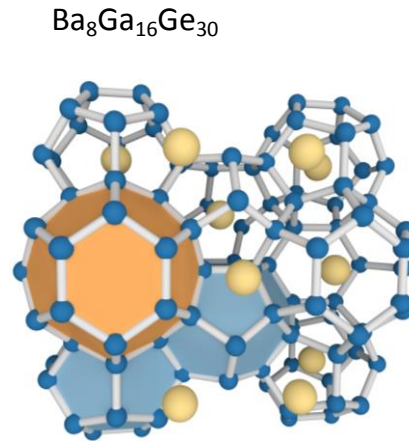


Vetenskapsrådet



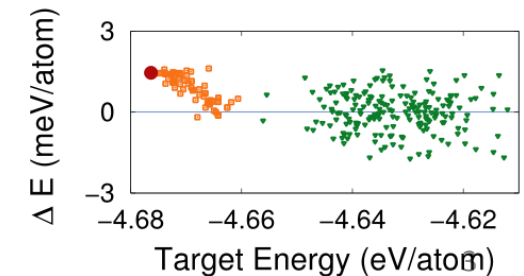
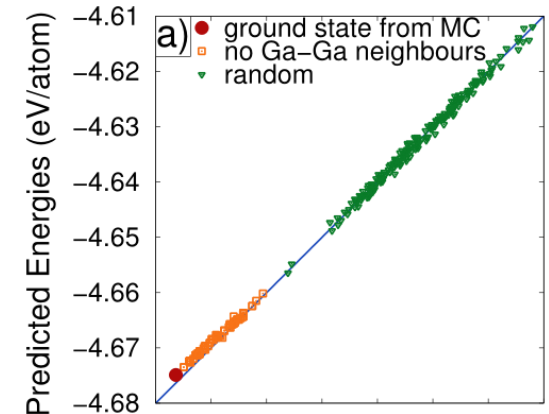
DFT calculations and cluster expansion

- Goals:
- Make IceT/MCHammer
 - 1. Sustainable software
 - 2. Available for ESS users



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

Ångqvist & Erhart, Chem. Mat.



Collaboration with DMSC

We can benefit from:

Contributions to:

- Molecular and Materials Modeling & Simulations
- Data analysis
- Automation
- Machine learning



We can offer:

Expertise on:

- Neutron scattering techniques and instrumentation
- Modelling and simulations
- Data analysis
- Software development and engineering
- Data infrastructure
- EU proposals and projects

We can expose your science to the ESS users

Any questions?



Global context for ESS Project



- 1996 – OECD setup a Neutron Sources Working Group as part of its Megascience forum
- 1998 OECD report – 3 major economic areas, USA, Japan, Europe should build new next generation neutron sources both for capacity & to replace older sources
- 2006 ESFRI (European Strategy Forum on Research Infrastructures) priority for ESS/neutrons 2010 roadmap update, 2014 priority to move forward
- Part of a suite of neutron and x-ray facilities for materials research

Facility	USA	Japan	Europe
High intensity x-ray synchrotron	Advanced Photon Source	Spring-8	European Synchrotron Radiation Facility (1)
Free Electron Laser pulsed x-rays	Linac Coherent Light Source	SACLA (FEL)	European XFEL (1)
High flux reactor neutron source	HFIR reactor	JRR3M reactor	Institut Laue Langevin (1)
High intensity spallation neutron source	Spallation Neutron Source	J-PARC (JSNS)	European Spallation Source (1,2)

(1) On the ESFRI roadmap, (2) Under construction