

SINE2020 General Assembly

Parma, 6 June 2018

WP 3

Training neutron scattering from proposal to publication

E-learning and schools

UCPH, DTU, STFC, CEA, MTA-EK

WP leader: Linda Udby, University of Copenhagen

Explanations of the work carried out

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



- Task 3.1: Development of e-learning platform
- Task 3.2: Development of a virtual neutron facility and training material
- Task 3.3: Enhancing coordination for Pan-European neutron training Schools



Task 3.1: Development of e-learning platform

- 3.1.1: Coordination & management
- 3.1.2: Server maintenance
- 3.1.3: Prospects of student interaction with material and assesment (D3.1)
- 3.1.4: Content development
- 3.1.5: Content collection and adaptation (D3.3)

Task 3.2: Development of virtual neutron facility

- 3.2.1: Development of virtual instrument models (D3.4)
- 3.2.2: Development of virtual experiment training material (D 3.7 & D 3.9)
- 3.2.3: Implement and test virtual experiments (D 3.9)

Task 3.3: Support for European neutron training Schools

- Support for introductory (D3.2 & D3.6 & D3.8) and advanced schools (D3.5) on neutron scattering (D3.10)

A little background-info for

Task 3.1 +2: Development of e-neutrons

- E-neutrons was founded by FP7 NMI3
- Contained an introductory neutron scattering course with outline of 10 modules.
- Need for further development of platform
- Need for further development of module and contents
- Need for ESS relevant material
- Need for more courses (advanced or neutron-related)
- Need for more virtual experiment training
- Need for more testing (pure online and blended-learning).

The screenshot displays the e-neutrons website interface. At the top, there's a navigation bar with links for FRONTPAGE, ABOUT E-NEUTRONS, FOR TEACHERS, and GET AN ACCOUNT, TIPS, SUPPORT. A search bar and login fields are also present. The main content area is divided into several sections:

- Courses:** Features a large banner for "INTRODUCTION TO NEUTRON SCATTERING - SELF STUDY" with a "READ MORE" button. Below it, there are smaller cards for "Introduction to Neutron Scattering" (High-guidance self study), "Introduction to Neutron Scattering" (Open course for blended learning), and "Muon Spin Spectroscopy" (A course on a complementary technique to neutron scattering).
- Science cases:** Includes cards for "Finding crystal structure" (Chemistry of materials), "Characterising liposomes in suspension" (Life sciences), "Characterising magnetic order" (Magnetic and electronic phenomena), and "Characterising atomic lattice vibrations" (Energy research). A "CRYSTAL STRUCTURE" section highlights a module on diffraction from crystalline materials.
- Exercise taster:** Shows a "Problem Fourier transform" section with a "FOURIER TRANSFORM" card asking "Do you know what the scattering intensity is from a string of particles? Test yourself here!" and a "READ MORE" button.
- Quiz taster:** Features a "NEUTRON PROPERTIES" card asking "Do you know what neutrons are good for and why? Test yourself here..." with a "READ MORE" button.
- Simulation taster:** Includes a "SMALL ANGLE SCATTERING" card asking "Do you know what the scattering pattern looks like from small particles in solution? Test yourself here..." with a "READ MORE" button.

Task 3.1.1: Coordination & management :

KPI#1: Statistics of website activity and computer performance. Our goal is to have at least per year

- 100 new users – (~200 last year – now 950 users)
- 3000 unique visits (~5400 last year)
- 6000 visits (~8600 last year)
- 95% uptime (~90 % last year – peak server overheat)
- support for 5 blended learning courses (6 last year)
- Data collection policy (GPDR)
- Access/ Support policy (under development)
- Recruitment



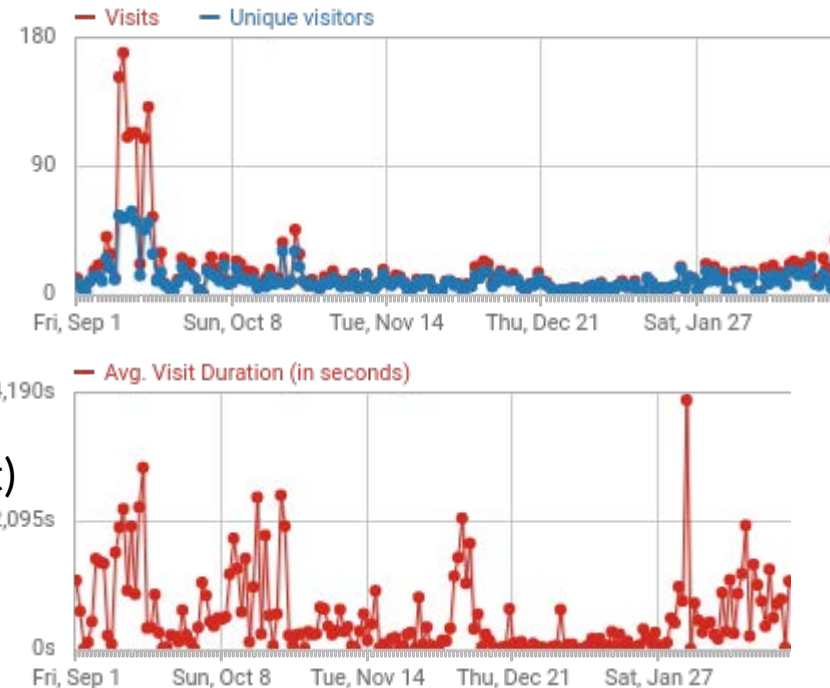
Tommy N W Ech-Knudsen
Student Assistant




Viktor L. Holm
Scientific Assistant



Mads Bertelsen
Post-doc



FRONTPAGE ABOUT E-NEUTRONS FOR TEACHERS SUPPORT

E-NEUTRONS DATA COLLECTION POLICY

When you create an account at e-neutrons you can rest assured that we will not pass on your personal information to third parties.

We do however use your anonymised registration data for reporting to our main sponsor (via the EU SINE2020 project). If you are enrolled in one or several courses at e-neutrons, the designated teachers and students of those courses at e-neutrons will have access to see your registration data.

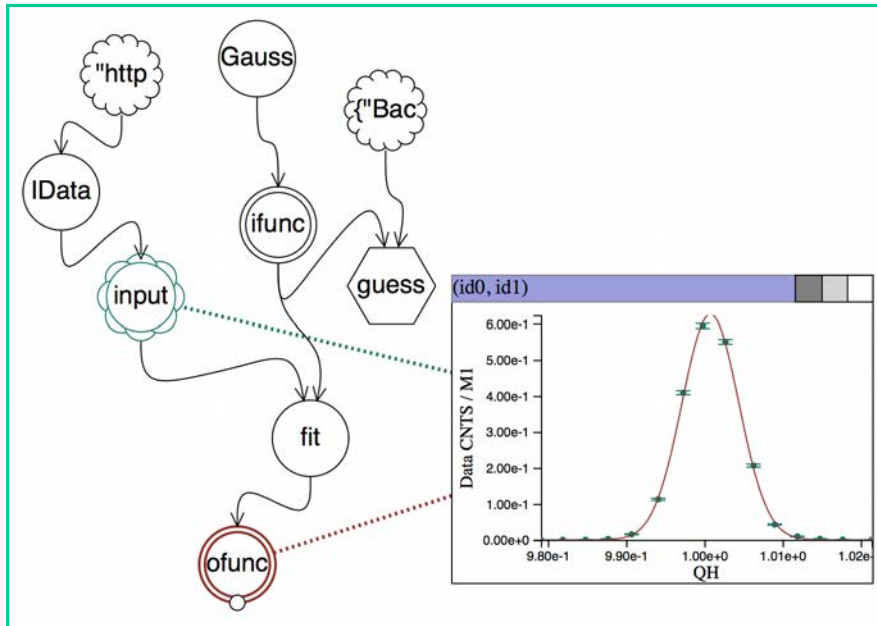
Since we are constantly working on improving the learning material at e-neutrons we log all sessions at e-neutrons as well as individual user progression in courses etc. We may use these data in non-profit didactical research projects in order to improve the content and structure of e-neutrons. If we do use your logged session-data it will only be for research purposes and we promise that it will always be in anonymised form.

If you have enrolled in one or several courses at e-neutrons, the designated teacher(s) of those courses will have access to track your progress within the course including attempts and grades in quizzes. Fellow students will not have access to track your progress including attempts and grades in quizzes.

By signing up to e-neutrons you certify your acceptance of the above data collection policy.

Task 3.1.2: Server maintenance and development

- Improvement of simulator: new 3D VR visualisation and webupload of files
- Cloning tool: developed to adapt open e-learning modules to closed classrooms
- IfitLab tool: Prototype solution for simple data analysis in the browser ([demo by Jakob Garde](#))



The screenshot shows the SimplePowderDiffractometer web interface. At the top, there is a navigation bar with the McStas logo, a 'Show menu' button, and a 'Logout' button. The main content area is divided into several sections:

- SimplePowderDiffractometer (click for documentation)**: A diagram showing the experimental setup with a source, collimator, sample, and detector.
- Parameters for SimplePowderDiffractometer**: A table of parameters and their values.

Parameter	Value	Description
lambda0 [Gaussian distribution]:	1	[AA] The mean value of incoming wavelengths (1)
diambda [AA]:	0.005	Gaussian sigma of incoming wavelength distribution (0.005)
coll [arcmin]:	120	horizontal collimation (120)
sample_can [1]:	0	When >0 a 2mm thick Al pressed powder can is inserted around the sample (0)
sample [1]:	Ni.laz	When >0 a 2mm thick Al pressed powder can is inserted around the sample (Ni.laz)
- Runtime configuration**: A table of runtime parameters.

Parameter	Value
neutron rays:	1000000
simulation steps:	1
random seed:	0
- Simulation**: A section showing the simulation parameters and results.

params: lambda0=1 diambda=0.005 coll=120 sample_can=0 sample=Ni.laz

neutron rays: 1000000

random seed: 0

simulation steps: 1
- Data plots (click here for log-scale)**: Two plots are shown. The left plot is a log-scale plot of 'Data CNTS / MI' vs 'QH' (0 to 100). The right plot is a 3D visualization of the detector geometry.

- **Task 3.1.3: Prospects of student interaction with material and assesment (D3.1)**
- Reviewed quizzes in open intro-ns course: type/reply/feedback/assessment options
Analysis of quiz questions in e-neutrons courses, 85 pages, Report UCPH (2018)
- Current quizzes designed for learning purposes. Mostly used in blended learning.
- If certification is wanted for online course alone, quizzes have to be re-designed, behaviour changed. Testing and maintainance needed for all user platforms.

Page 1

- 1 A simple virtual powder
- 2 Intensity at the detector
- 3 Varying the incoming wave
- 4 Relation between neutron wavelength and intensity
- 5 Varying the incoming neutron wavelength
- 6 Intensity of the diffraction pattern
- 7 Sample influence of intensity

Page 2

- 8 Diffraction from sample
- 9 Investigate the powder
- 10 Usefulness of sample container
- 11 Reciprocal lattice of Ni
- 12 Indexation of peaks

Page 3

- 13 Activity evaluation quiz

Question 8
Not complete
Marked out of 1.00
Flag question
Edit question

Do the diffraction patterns look the same with and without sample container? If not what are the differences? Select the most appropriate choice from your observations in your simulation with the container

Select one:

- ☐ The peaks have increased intensity
- ☐ The peaks change position
- ☐ There are new peaks
- ☐ The peaks are broader

☒ Check

Question 9
Not complete
Marked out of 1.00
Flag question
Edit question

In which diffraction experiments do you think simulation of the sample container would be useful? Select the most appropriate answer below

Select one:

- ☐ To simulate experiments which are carried out in a sample container
- ☐ To estimate whether using a sample container in the experiment will be problematic for the analysis of data from my sample
- ☐ To estimate the amount of sample needed to get a much bigger signal from that than from the container
- ☐ In experiments where I would like to separate the scattering data from container from scattering data from the sample
- ☐ all of the above

☒ Check

Information
Flag question
Edit question

At this point we would like to start interpreting the diffraction pattern in terms of a sample model.
If you are not already familiar with the realspace and reciprocal space model of Ni - it is probably useful for you to solve the quiz Reciprocal lattice of Ni before proceeding.

Question 10
Not complete
Marked out of 1.00
Flag question
Edit question

Drag the Miller indices to the corresponding peaks. The crosshair should be on the peak position.

☒ Check

Answers

Choice 1

There are new peaks

Grade: 100%

Feedback

We agree. The new peaks occur because the container is produced from another powder than the sample.

Choice 2

The peaks are broader

Grade: None

Feedback

We don't agree

Choice 3

The peaks change position

Grade: None

Feedback

We don't agree. The peaks from the sample are still in the same place but some new ones have also appeared

Choice 4

The peaks have increased intensity

Grade: None

Feedback

We don't agree. The peaks from the sample still have the same intensity but in addition some new peaks have also appeared

Task 3.1.3: Prospects of student interaction with material and assesment (D3.1)

Evaluation of student use of wiki through network analysis

Network analyses of student engagement with on-line textbook problems, 72 pages, Subm. Computers & Education (2018)

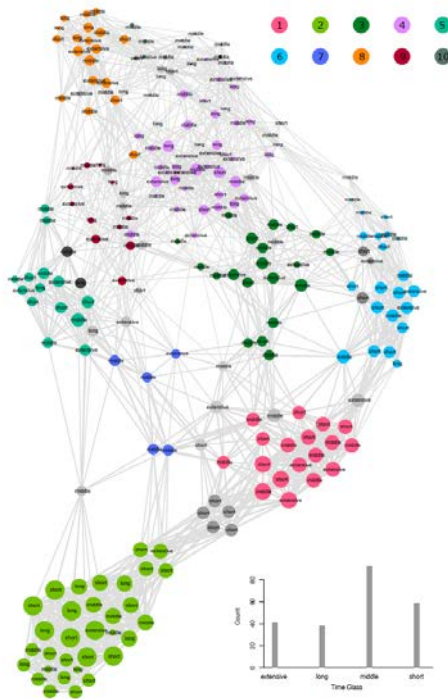


Figure 4: The sparsified similarity network. We have found 10 overlapping groups. Colors represent clusters, links represent similarity in the space of rotated components. Labels represent time classes found by analysing length of sessions. The inset shows the distribution of time classes for all problem solving sessions, see Section 6.4. Grey circles belong to more than one cluster.

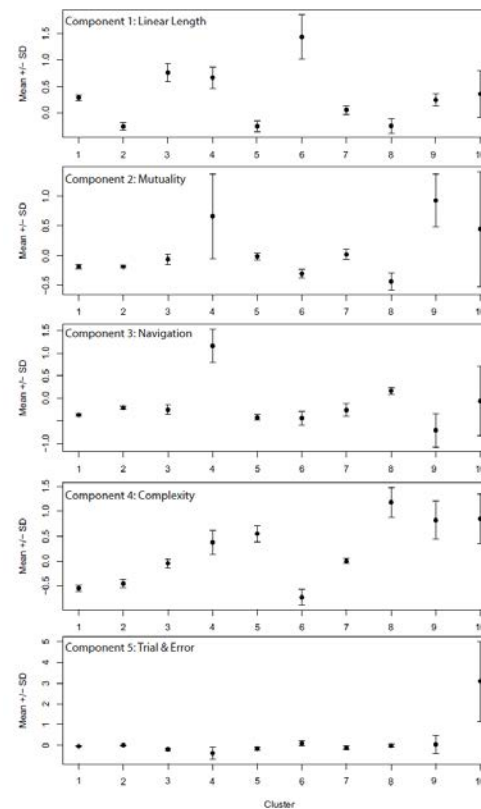


Figure 5: Mean component scores per cluster. Error bars represent 95% confidence intervals.

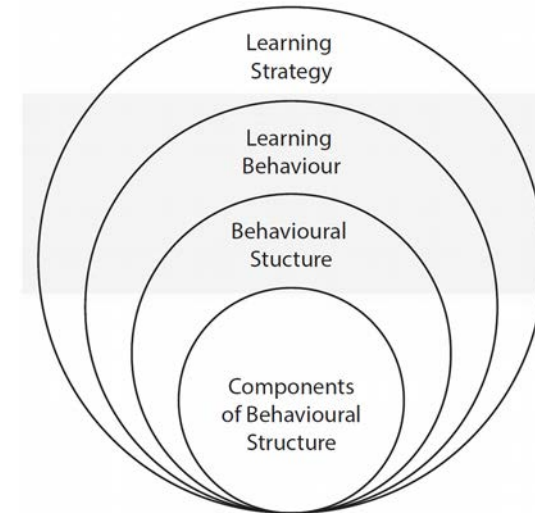


Table 6: Per cluster distributions of duration categories in clusters with significant Segregation on duration categories.

Cluster	Short 5-25 min.	Middle 25 min.-1.4h	Long 1.4-3h	Extensive 3h+	Sum
1	0.46	0.36	0	0.18	1
2	0.45	0.26	0.23	0.06	1
3	0.18	0.64	0	0.18	1
4	0.14	0.34	0.30	0.21	1
6	0.48	0.39	0.04	0.09	1
All	0.26	0.40	0.16	0.18	1

Task 3.1.4: Content development (D3.3)

- Intro-ns (open): 10 topics – 2 still under construction (~100 h)
- Intro-musr (open): 6 topics (+2) (~24 h). Ongoing collaboration with WP 10 development of Mantid e-learning.

Presented by Claire Wilde and Peter Baker.

- New (open) course “Advanced topics in Neutron Scattering” under construction. Each module/topic stand-alone (~4-10h) but build on intro-ns knowledge. Material to some modules expected to be contributed from e.g. other WPs
- Support and development of tailored e-courses connected to schools. Restricted access is needed for teachers to have access to edit material and see student answers etc.
- LU gave 2d hands-on workshop oct 2017 at ILL to 11 teachers (HERCULES school) on how to construct learning material at e-neutrons

Task 3.1.5: Content collection and adaptation (D3.3)

- (ongoing) Material (text format) from all SINE2020 supported schools available in Library
- (ongoing) Updating text-material in WIKI. Implementing hints and solutions to exercises.
- (ongoing) Further development of „Introduction to Muon Spin Spectroscopy“. Expanding to „7 aspects of muons“. Good collaboration with WP10 to develop e-learning material for Mantid.

Library

Dashboard / Courses / lib

Learning material used

- News forum
- Social forum
- Neutron WIKI textbook
- Live simulation site

Links to Databases

Reviews and Handi

Neutron Scattering

A collection of theoretical books and

Lecture Notes in Ph

This is a collection of conference pr

School: Neutron Sc

Annual research-based blended-lea

Topics: Introduction to neutron scat

Prerequisites: Undergraduate cour

Knowledge of crystallography is pre

Period: 7 weeks in class (Septemb

Credits: 7.5 ECTS

Assessment: Pass/fail of reports b

Contact: Kim Lehmann -lehmank@r

School: Berlin Scho

Cosmic Ray Muons

Dashboard > Cosmic Ray Muons > 02 Setting up a Cosmic Ray Experiment > Quiz 02

QUIZ NAVIGATION

Question 1 [edit]

Consider first a point source which emits flux Ψ_0 [cts/(s·ster)]. Calculate the inte

Solution

Question 2 [edit]

Consider now a moderator of a typical useful size of $150 \times 150 \text{ mm}^2$. The mod (cts/(s·m²·ster)). A beam port (slit) of size $50 \times 50 \text{ mm}^2$ is placed 4 m from the downstream from the beam port. Calculate how the neutron flux through dA va

Hint

The variation in distance between any point of the moderator and any point of

Hint

At a certain position (L') of dA , the beamport it starts to block part of the view

Solution

In the following the width and height of the square moderator is denoted d_m an square beamport denoted d_b . For $L < L'$ (case A, underilluminated beam port the beamport, but for $L > L'$ (case B) the moderator is shielded by the beam integrated intensity radiated in dA from a source with area A_m is

$$I = \int dA_m \int d\Omega \Psi_0 = \int dA_m \int dA \frac{\Psi_0}{L^2} = A_m \Delta A \frac{\Psi_0}{L^2},$$

where variations in the distance from different places on the source to the poi then

$$\Psi = \frac{I}{\Delta A} = A_m \frac{\Psi_0}{L^2},$$

Inserting a beamport does not change the flux for $L < L'$.

$$\Psi_{L < L'} = A_m \frac{\Psi_0}{L^2} = d_m^2 \frac{\Psi_0}{L^2} = 0.0225 \frac{\Psi_0}{L^2},$$

where L is the distance from the source (moderator) with area.

The flux at $L \geq L'$ is

$$\Psi_{L > L'} = A_b^2 \frac{\Psi_0}{L^2}$$

$$= (d_b^2) \frac{\Psi_0}{L^2}$$

$$= d_b^2 \left(\frac{L}{L - L_{port}} \right)^2 \frac{\Psi_0}{L^2}$$

$$= d_b^2 \frac{\Psi_0}{(L - L_{port})^2}$$

$$= 0.0025 \frac{\Psi_0}{(L - 4)^2},$$

since the beamport 'shields' the moderator giving an effective source size of $(d_b^2)^2$, i.e. effectively the detector (dA) sees a virtual source of size $(L_{port})^2$ at distance $L \rightarrow L_{port}$. The flux is plotted in Figure 2.

Figure 2: The flux Ψ [cts/(s·ster)] as a function of the distance L [m] from the source to the detector. The flux is plotted in Figure 2.

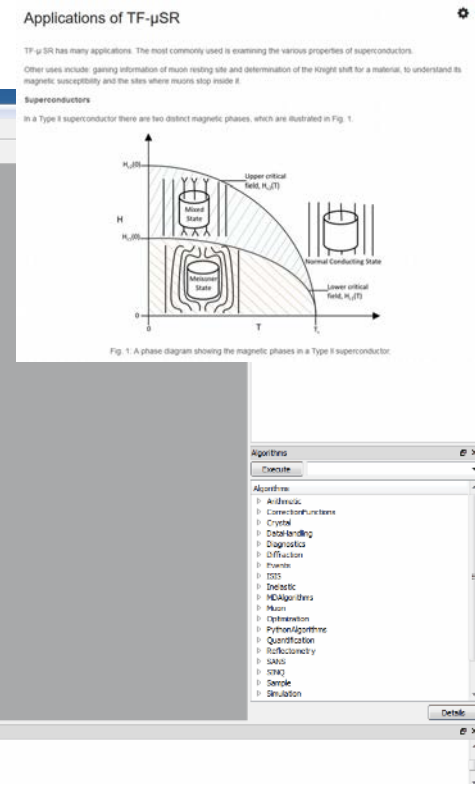
Applications of TF- μ SR

TF- μ SR has many applications. The most commonly used is examining the various properties of superconductors. Other uses include: gaining information of muon landing site and determination of the Knight shift for a material, to understand its magnetic susceptibility and the sites where muons stop inside it.

Superconductors

In a Type II superconductor there are two distinct magnetic phases, which are illustrated in Fig. 1.

Fig. 1: A phase diagram showing the magnetic phases in a Type II superconductor.



Algorithms

Execute

Algorithms:

- Arithmetic
- Correction systems
- Crystal
- Data handling
- Diagnosis
- Diffraction
- Points
- DSO
- Dynamic
- MDA algorithms
- Python
- Optimization
- Pyromagnetic
- Quantification
- Reflectometry
- SAS
- SWR
- Simulation

Script Interpreter

Python's own help system.

object -> details about 'object', use 'object()' for extra details.

help -> A brief reference about the graphical user interface.

•Task 3.2: Development of virtual neutron facility

KPI#2: Number of virtual instrument/experiments provided. Our goals are

- to have all instruments in the McStas software package available online (now 90%)
 - to develop tailored virtual instruments and virtual experiment exercises for at least 5 ESS relevant instruments (now identified)
-
- 3.2.1: Development of virtual instrument models (D3.4)
 - 3.2.2: Development of virtual experiment training material (D 3.7)
 - 3.2.3: Implement and test virtual experiments (D 3.9)
-
- Most work postponed to PR2+ PR3 due to maternity leave of LU & JH in PR1 . Furthermore JH left project unexpectedly in PR2. Catching up by extra recruitment in PR3 UCPH (2018-2019) and CEA (expected 2018-2019)

3.2.1+2: Development of virtual instrument models and training material (D3.4 + D 3.7)

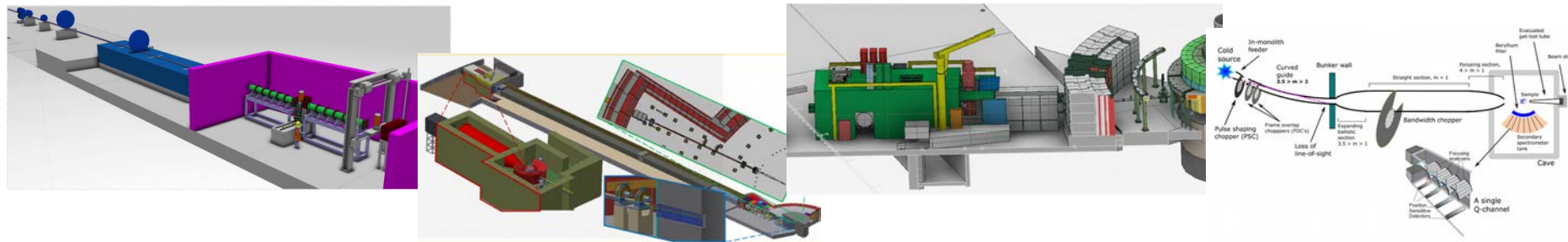
- We have decided to select 4 ESS relevant science cases & instruments covering a broad range of scientific fields. Tentatively

UCPH+DTU

- Cultural heritage sample investigated by (Bragg edge) imaging @ ODIN
- Formation of nanomagnets investigated by SANS&diffraction @ HEIMDAL
- Lipid exchange in nanodiscs investigated by SANS @ LOKI
- (Spin excitations in a HTSC investigated by INS @ BIFROST)

CEA

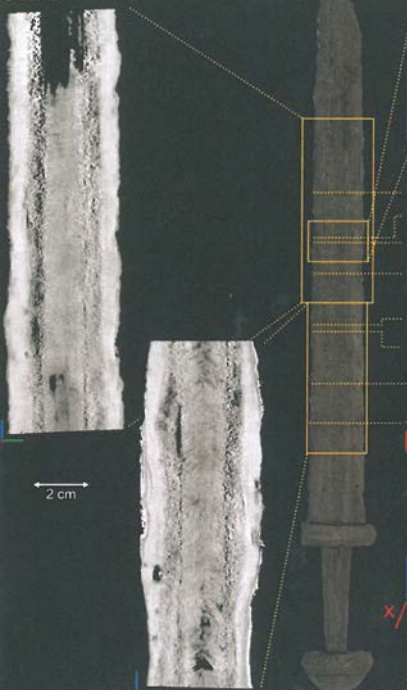
- Single crystal structure investigated by polarised diffraction @MaGIC



•3.2.1+2: Development of virtual instrument models and training material (D3.4 + D 3.7)

- For each case an outline and learning objectives (LO) will be decided and written
- Simple McStas virtual model of instrument, test simulated data versus LO
- Iterate on virtual instrument, simplify input parameters to comply with LO
- Implement as quiz or lesson at e-neutrons

C6375



Introduction:

The national museum director has been offered two viking age swords eye-inspection and both of them are offered as the rare Ulfberth sword. But the museum director suspects that one of the swords is a contemporary sword. One way to distinguish, is to see whether the core of the sword real Ulfberth sword would not be. But how to analyse the interior of it? Neutron Bragg edge imaging can distinguish between two different materials.

Student Task:

There are two viking-age swords A & B :
Sword A is a Ulfberth sword which is made fully cast from steel
Sword B is a contemporary copy welded from soft iron but with steel
Both have Ulfberth engravings close to hilt in pictures, but simulation engravings.

The task of the student is to decide which of the swords is the Ulfberth edge imaging data in the form of transmission pictures and analysis of neutrons from the sword core and edge, respectively.

Sword A will not show a difference in the ToF features/peaks between Sword B will show a difference between the ToF features/peaks between material is different.

Details in construction of the simulation

The swords models A and B will first be simulated as a rectangular box two triangular prisms of PowderN as the edges.

Soft iron is also called ferrite (alpha-Fe) with a bcc structure. We will A: powder of alpha-Fe in bcc structure

Steel is a microdomains of strained ferrite and cementite (Fe_3C). We will B1: powder of alpha-Fe with slightly expanded lattice parameter

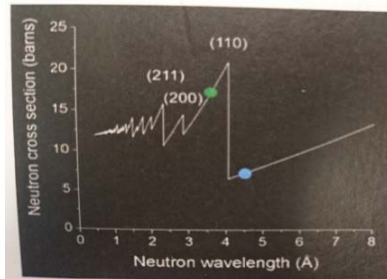
B2: powder of Fe_3C .
Realistically there would be only 10% B2 in a steel sample from that increase that in order to see an effect in the simulations.

We will first try to get the Absorbance versus wavelength of sword material to see a difference and explain the difference.

Then we will transfer the samples to a ToF simple instrument (short pulse) gradually change the instrument to be more ODIN-like.

Test 1a : See if we can reproduce total neutron cross-section versus wavelength curves from the reflections in bcc Fe gives absorption edges in the transmission curve. The absorption edge at wavelengths where a Bragg-peak would back-scatter neutrons ($2\theta = 180^\circ$).

Instead of the measured neutron transmission sometimes $1 - \text{transmission} = \text{absorption}$ is plotted; more directly comparable to the total neutron cross-section as shown below.



Ferrite total neutron cross-section, from Annas thesis page 124

Test with PSI-DMC powder diffractometer with following changes

```
SPLIT 10 COMPONENT sample = PowderN (
  d_phi=D_PHI, radius=sample_radius, yheight=sample_height, DW=Dw,
  pack=PACK, reflections = filename, barns=BARNs, p_transmit=0.5, p_inc=0)
AT (0, 0, 0) RELATIVE sa_arm
```

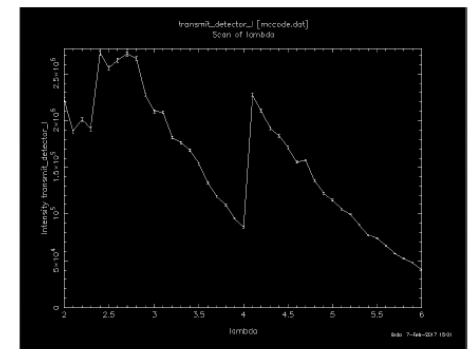
```
/*COMPONENT STOP = Beamstop(radius=0.3)
AT (0,0,1.4) RELATIVE sa_arm
ROTATED (0,0,0) RELATIVE sa_arm */
```

```
COMPONENT Detector = Monitor_nD(
  xwidth=3.0, yheight=0.09, filename="detector.dat", min=19.9+SHIFT, max=179.9+SHIFT, t
  // max=99.9
  options="banana, theta", restore_neutron=1)
AT (0,0,0) RELATIVE sa_arm
ROTATED (0, 0, 180) RELATIVE sa_arm
```

```
COMPONENT transmit_detector = PSD_monitor(
  filename="PSD_detector", restore_neutron = 1, filename = transmit_detector, xwidth = 0.005,
  yheight = 0.01)
AT (0, 0, 0.02) RELATIVE sa_arm
```

The idea of the small transmit detector to scan the incoming wavelength and then we should be able to see a pattern which is inversely proportional to the total neutron cross-section versus wavelength.

Simulation: reflections=Fe.lau. All reflections have the same scattering cross-section 3.57210 barns since alpha-Fe is bcc.
We scan $\lambda = 2.0-6.0$, the result is shown below.



We observe a dip in the transmitted intensity at 4Å corresponding to the (110) ferrite reflection which would backscatter $2\theta = 180^\circ$ at $\lambda = 4.06$ Å.

We furthermore observe a dip at 2.3 Å. The closest lying back-scattering reflection would be the (200) which should backscatter at 2.86 Å, so we don't know why the absorption edge λ is so low. The multiplicity of (110) is 12 but of (200) it is only 6 so we expect a larger dip for the former edge, which corresponds well with data.



- Task 3.3: Support for European neutron training Schools

To be presented by Alain Menelle

SINE2020 WP3 Support for neutron schools

- Guarantees the availability of grants, therefore the **participation of students from other regions/countries** without neutron sources
- Helps to **grow the neutron/muon community** and recruits new users from various fields
- Helps to pass knowledge and experience about specific methods that often can not be reached in other ways
- Some of the **schools could not be organized without the SINE2020 support**

SINE2020 WP3 development of e-neutrons

- Will provide a **full course on neutron scattering where anyone can enroll for free. Would not be possible without SINE2020 support.**
- Will make neutron experimentation readily available even **for students who cannot attend hands-on training**
- Will provide easy accessible e-training elements involving a broad range of science cases which may **attract new users to neutron community and ESS**
- Will make it easier for students to transfer knowledge between neutron techniques by carrying a single science case through several quizzes.
- With course on muon spin spectroscopy, **synergy will be enhanced between the fields (NS and muSR).**
- Will provide an **e-learning sand-box for each hand-on school** in which teachers/organisers can freely adapt e-learning material from intro-ns course. We expect that schools will also contribute material back to e-neutrons.
- Has opened the possibility to develop an introductory x-ray course based on virtual experiments (similar to the introductory neutron scattering course). If pursued it will increase awareness of neutrons in xray community and vice versa. Possible to make a joint xray/neutron course targeted for e.g. industry. Implementation needs funding however.

Schools

- D 3.5. Advanced schools: Some budget unspent due to lack of organisers. Suggest transfer of remaining budget to develop more advanced e-learning modules based on virtual experiments instead (shift budget to reinforce D 3.4 + D3.7)
- Little or no participation at the schools from industrial field:
Exhibition window by e-learning animations from WP4 may provide a stepping stone.
- Difficult to reach and rise interest towards neutron and muon trainings outside of Universities and Research Centres (exception: archaeological field)

E-learning

- D 3.1 : Investigation of e-learning tools: **Delivered** (delayed to M30)
- D 3.3. Prospects of muon e-learning: **Delivered** (earlier than expected). Will however continue to develop muon e-learning course further during PR3
- D3.4+3.7 : Development of virtual instruments and training material:
Delivery **postponed** to M40-48 to give time to recruit and expand scope by transfer from Adv. Schools unspent budget (see D 3.5).