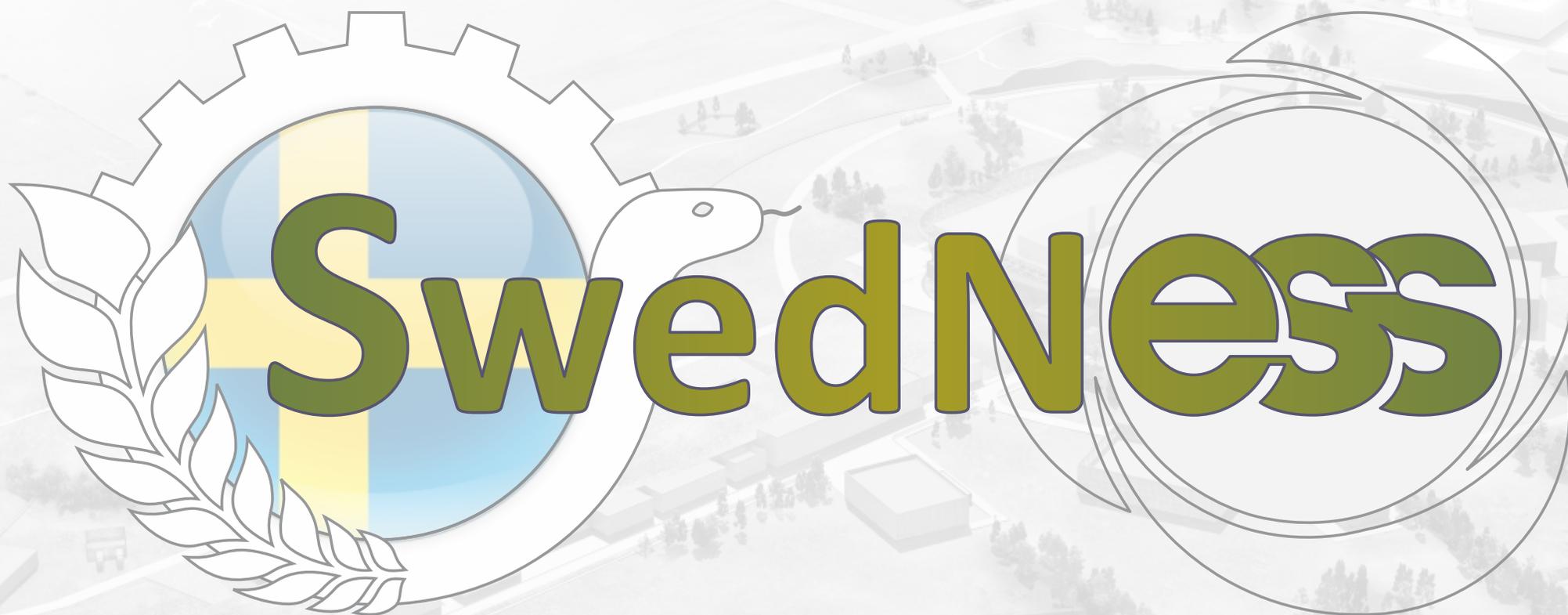


**SwedNess**



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Swedish Neutron Education for Science & Society

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# SwedNess

- Swedish national graduate school in neutron scattering
- Collaboration between 6 of Sweden's biggest academic institutions:

**CHALMERS**



**LUND**  
UNIVERSITY



UPPSALA  
UNIVERSITET



Linköping  
University



Stockholm  
University



- Fully funded by the Swedish Foundation for Strategic Research (SSF), which main goal is to strengthen Sweden's future competitiveness in science, engineering and medicine.
- Bridge between fundamental research and industry).
- Budget 120 MSEK (+100 MSEK) with 20 (+20) PhD Students



SWEDISH FOUNDATION *for*  
STRATEGIC RESEARCH



# SwedNess - Aims

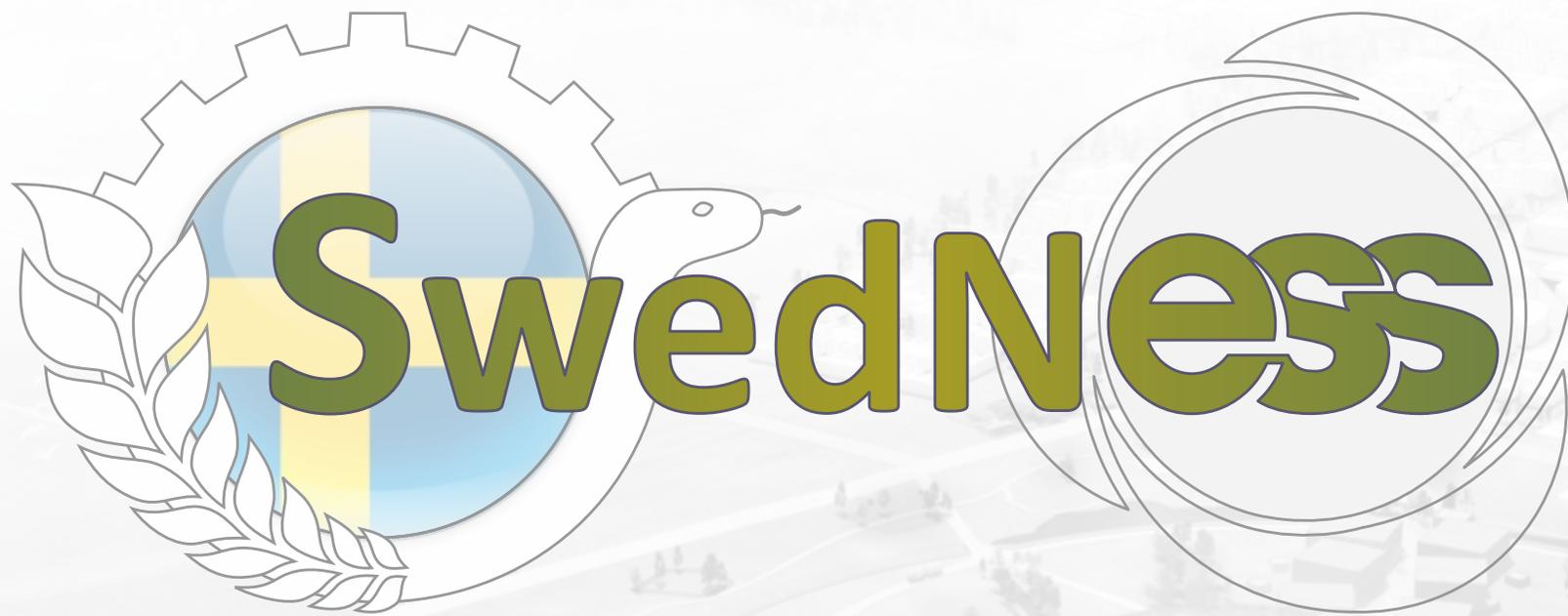
- To expand and broaden the **Swedish neutron scattering community**.
- To support the six participating universities to take **full advantage of the ESS**
- To broaden the national scientific impact by involving **universities outside the alliance** in courses and research projects within SwedNess.
- To perform **excellent research** using NS within four research themes: Functional Materials, Life Sciences, Engineering and Basic Physics/Chemistry
- To promote **interdisciplinary** activities between such research themes.
- To create a strong academic collaboration & networking with **Swedish industry** in the use of neutron scattering.



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- To be a strong partner in the **Nordic neutron scattering community**





**NNSP**

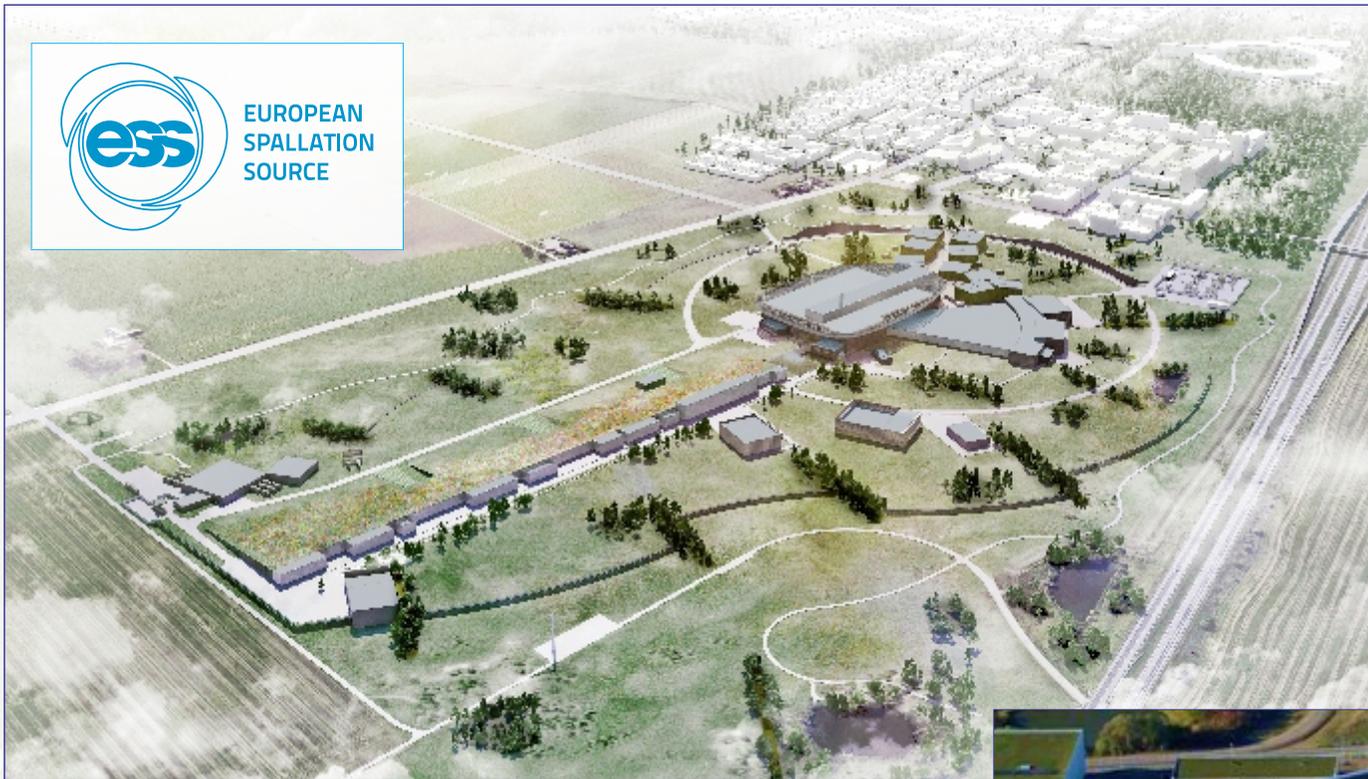


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- To promote **interdisciplinary** activities between such research themes.
- To create a strong academic collaboration & networking with **Swedish industry** in the use of neutron scattering.
- To be a strong partner in the **Nordic neutron scattering community**
- To broaden the international scientific impact by collaborating with **Baltic & international institutions**.
- To promote and plan for the complimentary use of **neutrons and x-rays**, especially in relationship to the co-location of **ESS and MAX IV**.



EUROPEAN  
SPALLATION  
SOURCE



**1.843 billion €uro**

**0.7 billion €uro**

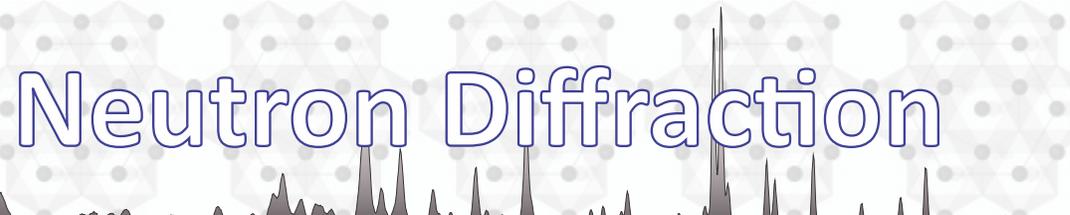




# Specialized Courses - SwedNess Course Catalogue



Neutron Diffraction



Feb./March 2020  
Stockholm University  
7.5 ECTS



Neutron Reflectivity & GISANS



~June 2020  
Uppsala  
3 ECTS



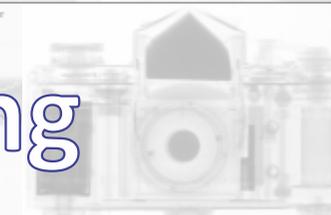
Small-Angle  
Neutron Scattering  
(SANS)



December 2019 (TBA)  
Lund University  
3 ECTS



Neutron Imaging



November 2019 (TBA)  
Lund University  
3 ECTS



Neutron Spectroscopy



December 2019 (TBC  
)Chalmers + ISIS  
5 ECTS

# Specialized Courses - SwedNess Course Catalogue



Engineering Materials  
Science using Neutrons

March - April 2020 (TBA)  
5 ECTS  
LiU (+ Chalmers & KTH)



Neutrons for Life Science

Spring 2020  
TBA  
Linköping Univ. (LiU)



Neutrons for the study of  
electrochemical processes

May 2020 (TBC)  
5 ECTS  
KTH + Uppsala Univ.

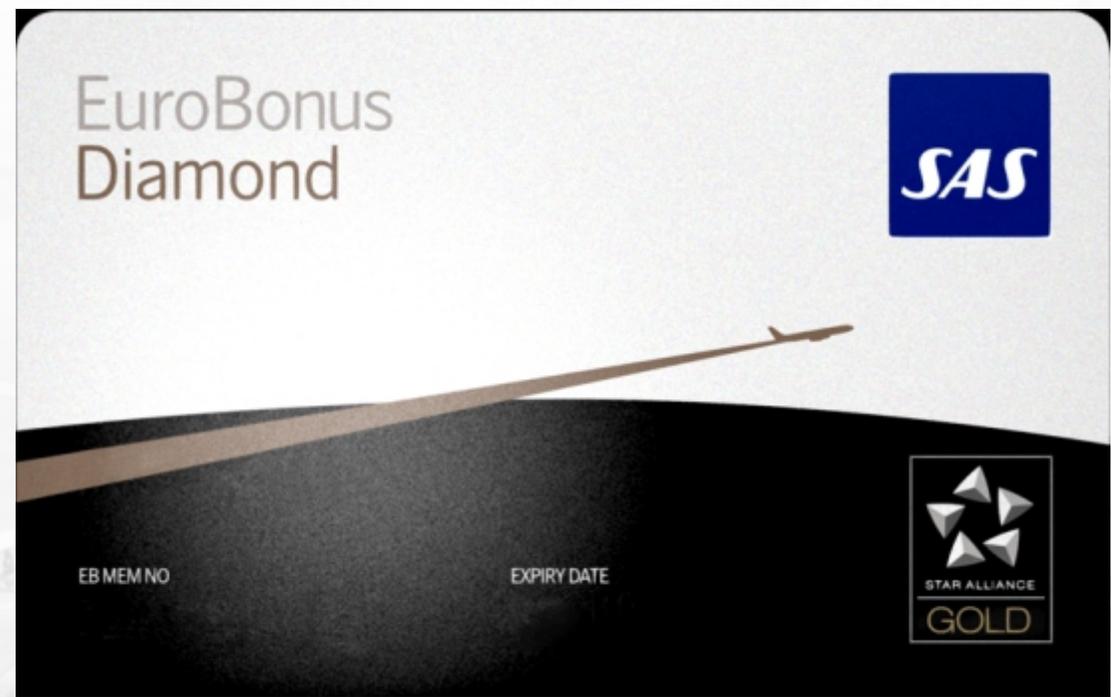


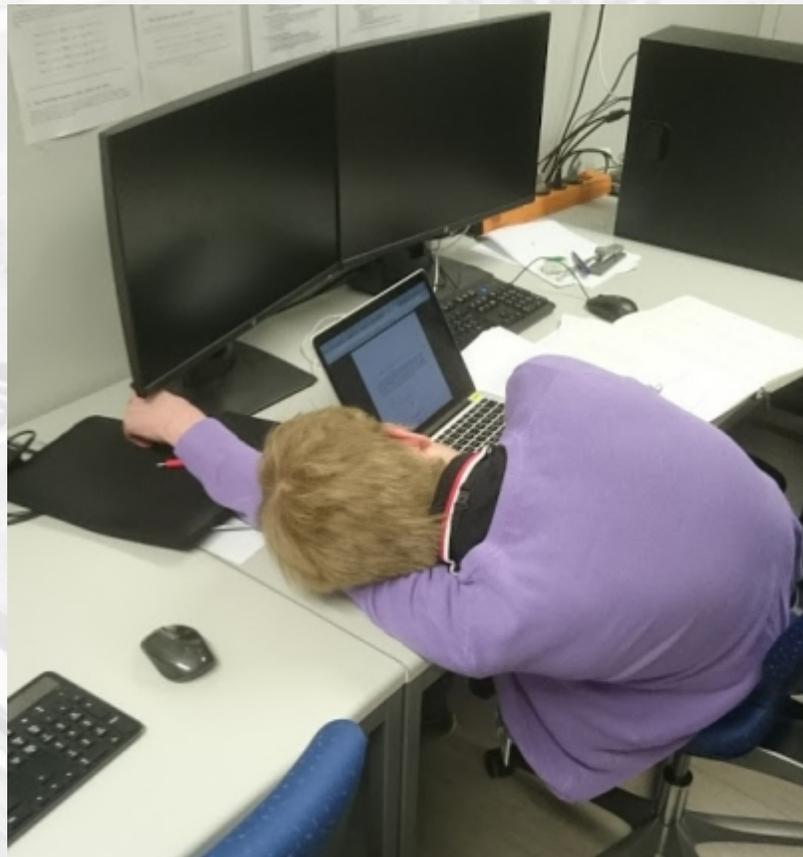
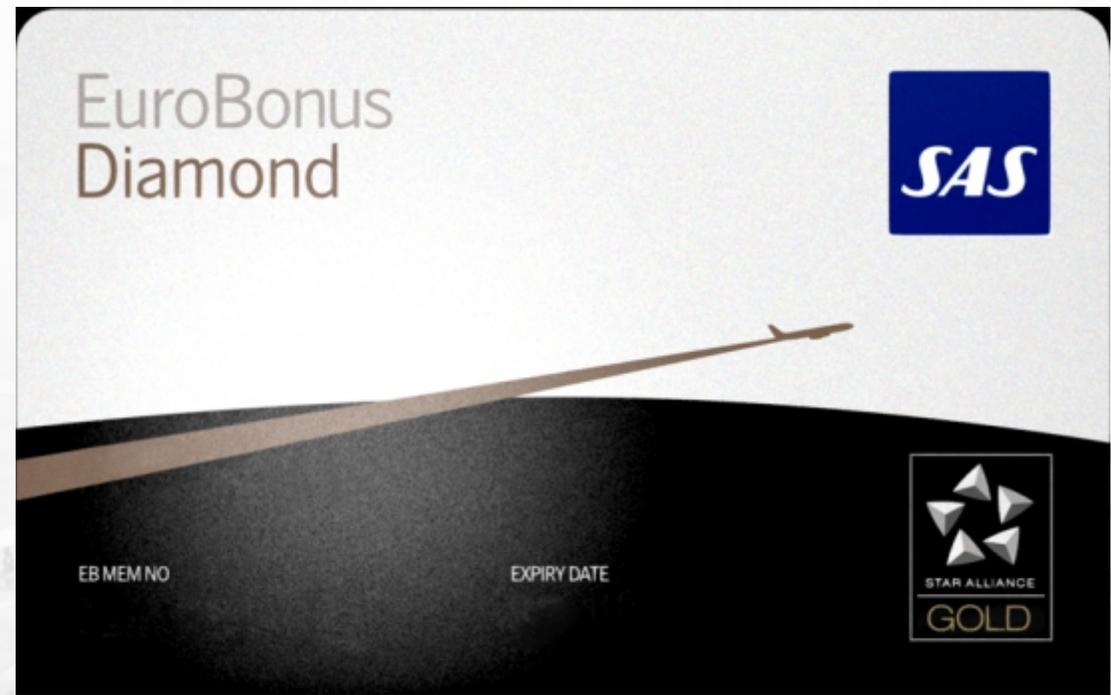
Neutrons & Muons  
for Magnetism

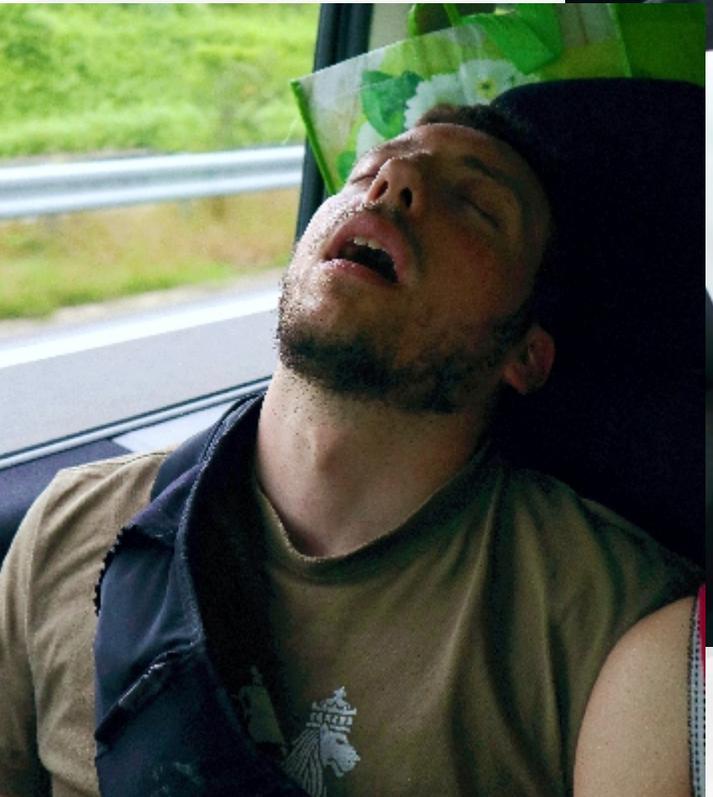
Spring 2020 (TBC)  
7.5 ECTS  
KTH, Stockholm

# Neutron Sources of the World









# Prepare for Beamtime = Proposal Writing

- Idea for how neutrons can help your research (specific question = piece of the puzzle)
- Talk to an expert (this will soon be You !!!)
- Consider your sample!!! (available size/mass, crystal/powder/thin film).
- Think about if you sample contains elements with low scattering or high absorption  
<http://www.ncnr.nist.gov/resources/n-lengths/>
- Select appropriate source & instrument for your experiment (**check deadlines + shutdowns!**)
- Contact instrument responsible to discuss experiment (**before you submit proposal!**)
- Write a proposal and apply for beamtime at your selected neutron source/instrument
- Cross your fingers and wait for the review committee + in some cases "national quota"
- If you obtain beamtime start to prepare your experiments well advance (align crystals, manufacture sample holders etc.)
- Check necessary paperwork (**visa!**) at source and perform the mandatory "safety training"
- If you plan to do experiments at different sources with same samples: consider activation of your samples (active sample transport is complicated and expensive!)

# Examination of this Course

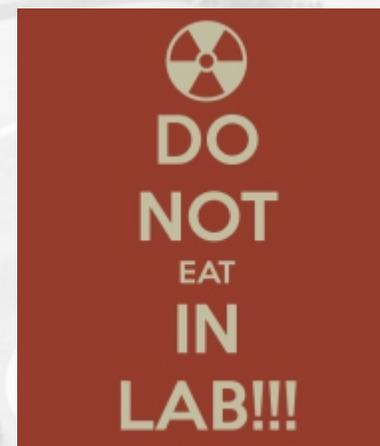
- You should all write a proposal for neutron beamtime
- Time during these 2 weeks and dedicated “finish up session” on 20 September.
- Submit to Me (Martin Månsson, [condmat@kth.se](mailto:condmat@kth.se)) by latest **29 September 2019**
- If you do not hand in the examination on time, you will **NOT BE REIMBURSED !!!**

A screenshot of the PSI Digital User Office website. The browser address bar shows the URL https://duo.psi.ch/duo/user\_new\_prop.php. The page title is "PSI Digital User Office". The user is logged in as "Prof. Dr. Martin Månsson". The main content area is titled "Proposal submission" and asks the user to select the PSI Facility for a new proposal. A table lists the facilities and their deadlines. A green thumbs-up icon is overlaid on the bottom right of the screenshot.

	Facility	Deadline (CEST)
Create new proposal	SLS - Swiss Light Source (Non PX)	15.09.2017 23:59:59
Create new proposal	SLS - Swiss Light Source (PX)	15.10.2017 23:59:59
Prepare new proposal	SINQ - Swiss Spallation Neutron Source	Currently no open call
Prepare new proposal	SµS - Swiss muon Source	Currently no open call
Prepare new proposal	Joint neutron - X-rays powder diffraction (SINQ and SLS)	Currently no open call

# Paper Work / Administration / Safety

- Depending on your nationality you might need a visa to visit some of the neutron sources around the world.
- Take this seriously and apply in time !!! Invitation letter from source (talk to respective user office) + letter from head of department. We could possibly also write something from SwedNess / NNSP...
- Always make sure you do the safety training before going to beamtime and follow the rules when you are there! This is your health we are talking about and... radiation safety officers do not usually have a sense of humor!!!
- Talk to your respective university about getting a “dose pass” to keep track of your total radiation dose during all of your experiments.



# Diffraction / Fullprof & Vesta (11 September)

1.

Download / Install the Fullprof suite + Exercises-dat (tutorials)

<https://www.ill.eu/sites/fullprof/>



Fullprof



## FullProf Suite Homepage

<https://www.ill.eu> > [sites](#) > [fullprof](#) > このページを訳す

The FullProf Suite (for Windows, Linux and macOS) is formed by a set of crystallographic programs (FullProf, WinPLOT, EdPCR, GFourier, etc...) mainly developed for Rietveld analysis (structure profile refinement) of neutron (constant ...

[Downloads](#) · [Programs](#) · [FullProf News](#) · [Examples & Tutorials](#)

## FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

[Introduction](#) · [What's new](#) · [Programs](#) · [Downloads](#) · [Examples & Tutorials](#) · [Support](#) · [References](#)

## Downloads

The FullProf Suite (for Windows, Linux and macOS) is formed by a set of crystallographic programs (FullProf, WinPLOT, EdPCR, GFourier, etc...) mainly developed for Rietveld analysis (structure profile refinement) of neutron (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle.

## FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

[Introduction](#) · [What's new](#) · [Programs](#) · [Downloads](#) · [Examples & Tutorials](#) · [Support](#) · [References](#)

Name:	Version date:	Platform:	File size:	Link:
FullProf_Suite Windows (32 bits, XP-compatible)	12 - July - 2019	Windows XP-7-10 (Last Supported Version)	91,681,889 bytes	<a href="#">Download</a>
FullProf_Suite Windows (32 bits)	11 - July - 2019	Windows 7-10	94,113,228 bytes	<a href="#">Download</a>
FullProf_Suite Windows (64 bits)	11 - July - 2019	Windows 7-10	104,545,007 bytes	<a href="#">Download</a>
FullProf_Suite Linux (64 bits)	12 - July - 2019	Linux - Intel	113,320,124 bytes	<a href="#">Download</a>
FullProf_Suite MacOS (64 bits, unsigned)	1 - October - 2018	macOS - Intel (Ago)	116,326,479 bytes	<a href="#">Download</a>
FullProf4Mac.app (64 bits, signed) - v2.5.4	18 - May - 2018	macOS - Intel (.dmg)	116,707,285 bytes	<a href="#">Download</a>

## FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

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### Available items in Catalogs section:

Name:	Description:	File size:	Link:
FullProf Manual	Users' Guide of FullProf	1,769,341	<a href="#">Download</a>

### Available items in Tutorials section:

Name:	Description:	File size:	Link:
Atlanta-doc	PDF-docs of a School in Atlanta	2,171,360	<a href="#">Download</a>
ECM-21-Workshop	PDF-docs of ECM-21 Workshop	1,055,669	<a href="#">Download</a>
Exercises-dat	Data files, FullProf exercises	54,250	<a href="#">Download</a>
Exercises-pcr	PCR files, FullProf exercises	35,608	<a href="#">Download</a>
HoCa_Tutorial	Tutorial magnetic structure	1,130,682	<a href="#">Download</a>
KTh3F12_Tutorial	Tutorial magnetic structure	501,244	<a href="#">Download</a>
Microstructural_effects	Documents about microstructure	544,914	<a href="#">Download</a>
pcr_dat	Data and PCR files	824,597	<a href="#">Download</a>
size-sph	Notes about size effects	14,298	<a href="#">Download</a>
sr_oxalate	Simulated annealing in FullProf	30,958	<a href="#">Download</a>

### Available items in Examples section:

Name:	Description:	File size:	Link:
FullProf examples	A set of PCR examples files to run on FullProf program	546,446	<a href="#">Download</a>

## Examples & Tutorials

- (1) Install Fullprof Suite
- (2) Download Exercises -dat



# Diffraction / Fullprof & Vesta (11 September)

2.

Download / Install the Vesta software:

<http://jp-minerals.org/vesta/en/>

Google

VESTA



VESTA - JP-Minerals

[jp-minerals.org](http://jp-minerals.org) > [vesta](#) > このページを訳す

2019/06/15 - VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. Some of the novel features of VESTA are listed below. Deal with multiple structural ...

VESTA  
Visualization for Electronic and Structural Analysis

Software > VESTA

### 1. Introduction

VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. Some of the novel features of VESTA are listed below.

- Deal with multiple structural models, volumetric data, and crystal morphologies in the same window.
- Support multiple tabs corresponding to files.
- Support multiple windows with more than two tabs in the same process.
- Deal with visually unlimited number of objects such as atoms, bonds, polyhedra, and polygons on isosurfaces (theoretical limit on 32bit operating system is 1,275,541,823).
- Support lattice transformation from conventional to non-conventional lattice by using matrix. The transformation matrix is also used to create repetitive and sub-lattice.
- Visualize interatomic distances and bond angles that are restricted in Rietveld analysis with RISTAN FP.
- Transparent isosurfaces can be overlap with structural models.
- Interface can be colored on the basis of another physical quantity.
- Arithmetic operations among multiple volumetric data files.
- High quality smooth rendering of isosurfaces and sections.
- Export high-resolution graphics images exceeding Video card limitation.

VESTA is a successor to two 3D-visualization programs, VICES and VIND, in the [VESTAS \(Visualization of Electron/Molecular and Structural\) software package](#).

VESTA runs on Windows, Mac OS X, and Linux. It is distributed free of charge for non-commercial users.

### 2. New features in VESTA 3

- Visualization of crystal morphologies
- Superposition of multiple structural models, volumetric data, and crystal faces on the same Graphic Area
- Visualization of isosurfaces with multiple levels
- An extended bond search algorithm to allow more sophisticated search in complex molecules, csg-like structures, etc.
- Calculations of electron and nuclear densities from structure parameters
- Calculations of Patterson function densities from structure parameters or volumetric data
- Integration of electron and nuclear densities by Voronoi tessellation
- Significant performance improvements in rendering of isosurfaces and calculation of slices
- Output information about principal axes and mean square displacements for anisotropic thermal motion
- Determination of the best plane for selected atoms
- Displaying labels of atoms

VESTA  
Visualization for Electronic and Structural Analysis

Software > VESTA > Download

### License agreement

VESTA LICENSE  
Version 3  
Copyright (C) 2006-2019, Koichi Momma and Fujio Izumi

This software is distributed free of charge for academic, scientific, educational, and noncommercial users. Users belonging to commercial enterprises may also use this software at no cost until a license for business users is established. Permission to use this software is hereby granted under the following conditions:

- 1) Drawings produced by VESTA may be used in any publications provided that its use is explicitly acknowledged. A suitable reference for VESTA is:  
[K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr., 44, 1272-1276 \(2011\).](#)
- 2) You should not redistribute any copy of the distributed files unless you have a written permission from us.

Part of these terms may be changed without any prior announcement.  
This software is provided "as is" without any express or implied warranty.

Please report bugs and help us improve VESTA.  
E-mail: [vesta.dev\(at\)gmail.com](mailto:vesta.dev(at)gmail.com)

If you want release announcements of new versions, subscribe to VESTA announce list.

Google Groups

Subscribe to VESTA announce

Email:

[Visit this group](#)

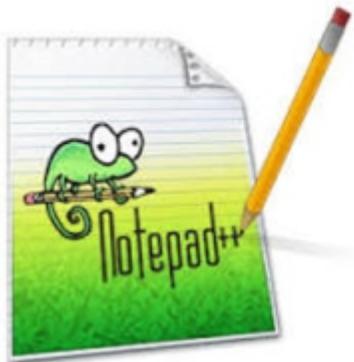
To unsubscribe, please email to the following address.  
[vesta-dev@googlegroups.com](mailto:vesta-dev@googlegroups.com)

NNSP



# Diffraction / Fullprof & Vesta (11 September)

3.  
Have a “good” text editor installed on your laptop



**Notepad++ : MS**



**TextWrangler: Mac**



## Modeling Magnetism / spinW

For the linear spin wave theory tutorial on Tuesday 17 September, a few softwares will be needed. Please try to complete the following preparations during the first week of the school.

- (a)** If you have access to a license, install Matlab  
<https://se.mathworks.com/products/matlab.html>  
Many universities provide student licenses. Do not worry if you do not have a license, we will work in groups at the tutorial and share computers with Matlab as needed.
- (b)** Install the spinW software for linear spin wave theory from  
<https://github.com/spinw/spinw/releases/tag/v3.1>  
For the installation, additional details can be found at  
<http://spinw.org/installation/>
- (c)** Register for an account on the Organic Materials Database (OMDB) on <https://omdb.mathub.io/>

# Quasi-Elastic Neutron Scattering (QENS) / Mantid

**For QENS Lecture / Exercise  
Wednesday 18 September  
Please download and install the  
latest version of Mantid 4.0.0**

**mantid**



**<https://download.mantidproject.org/archives.html>**

# Change of Venue for Lectures / Exercises



**18-20  
September**

**Tartu Loodusmaja  
Lille 10  
51010 Tartu**

