Welcome to the NNSP/SwedNess Intro Course in Neutron Scattering

As. Professor Martin Månsson - KTH Royal Institute of Technology - condmat@kth.se

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Why Give this Course?

- Neutron scattering is a optimal and very versatile technique to study materials, devices and objects.

- Neutrons are unique in several aspects and are able to directly probe some things other techniques can not.

- Neutron scattering techniques cover a very broad scientific scope.

Why Give this Course?

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1.843 billion €uro

0.7 billion €uro

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The School Program

Week 1

Time / Date	Morning Session I 08:30 – 10:00	Morning Session II 10:30 – 12:00	12:00 - 14:00	Afternoon Session I 14:00 – 15:30	Afternoon Session I 16:00 – 17:30
Mon 18 Oct					
Tue 19 Oct					
Wed 20 Oct	**L0 "Welcome"** • Course information • Examination Procedure **Martin Månsson, KTH**	**L1 "Course Overview"** • The Neutron/scattering experiment • Neutron Technologies • Elastic/Inelastic • Brief overview of the techniques **Martin Månsson, KTH**	Lunch	**L2.1 "Intro"** • Basic interaction mechanism (+x-rays) **Kim Lefmann, NBI** (Recorded Lecture)	**L2.2 "Intro"** • Scattering from 1 & 2 Nuclei • Coherent / Incoherent **Kim Lefmann, NBI** (Recorded Lecture)
Thu 21 Oct	**L2 "Neutron Sources & Technology"** • Sources Moderators • Monochromators / choppers • Collimation / Filters / Guides • Detection **Kim Lefmann, NBI**	**Ex. 1** • Wiki problem: Pinhole collimation • Quiz: Neutron detection • Quiz: Test your knowledge of neutron sources and instrumentation **(e-learning)**	Lunch	**L3 "Neutron Interaction with Matter"** • Cross Section, Isotope Sensitivity • Elastic / Inelastic • X-rays/electrons • Multiple Scattering **Kim Lefmann, NBI**	**Ex. 2** • Quiz: The neutron cross section • Wiki problem: Selection of materials **(e-learning)**
Fri 22 Oct	**L4 "Magnetic Scattering"** • Magnetism • Nuclear/Magnetic Scattering **Kim Lefmann, NBI**	Catch up on assignments and inquire about things you did not understand.	Lunch	**L5 "Crystallography"** • Crystallography • k-space **Magnus H. Sørby, IFE**	**Ex. 2 "Reciprocal lattice of Ni"** • Quiz: Reciprocal lattice of Ni **(e-learning)**
Sat 23 Oct	Free Weekend				
Sun 24 Oct	Free Weekend				

The School Program

Week 2

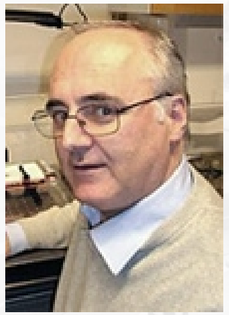
Time / Date	Morning Session I 08:30 – 10:00	Morning Session II 10:30 – 12:00	12:00 - 14:00	Afternoon Session I 14:00 – 15:30	Afternoon Session I 16:00 – 17:30
Mon 25 Oct	**L6 "Diffraction I"** • The Rietveld Method **Magnus H. Sørby, IFE**	**Ex. 3** • Simulation quiz: Diffraction from powder **(e-learning)**	Lunch	**L7 "Diffraction II"** • Instrumentation • Total Scattering **Magnus H. Sørby, IFE**	**Ex. 4** • When is Xray or Neutron diffraction suitable? • Wiki problem: Bragg scattering from non-Bravais lattices **e-learning**
Tue 26 Oct	**Ex. 5: TUTORIAL Fullprof Refinement I Magnus H. Sørby, IFE**	**Ex. 6: TUTORIAL Fullprof Refinement II Magnus H. Sørby, IFE**	Lunch	**L8 "Reflectometry I"** • Instrumentation • Specular/off-specular • Optical Matrix • Kinematic Approximation • Applications **Adrian Rennie, UU**	**Ex. 7** • Simulation quiz: Reflectometer • Optical matrix fits **e-learning**
Wed 27 Oct	**L9 "Reflectometry II / GISANS"** • Distorted Born approximation • GiSANS Instrumentation • In plane / out of plane • Applications **Adrian Rennie, UU**		Lunch	**L10 "Imaging"** • Instrumentation • Radiography / Tomography • In operando • Neutrons / x-rays **Luise Theil Kuhn, DTU**	**Ex. 8** • Simulation quiz: Bragg Edge Imaging on Viking Sword **e-learning**
Thu 28 Oct	**L11 "SANS I"** • Instrumentation • Scattering Length Density • Form-/Structure Factor • Approximations **Andrew Jackson, ESS/LU**	**Ex. 9** • Simulation quiz: Small Angle Neutron Scattering • Resolution (wavelength vs. angle) • Data Treatment **e-learning**	Lunch	**L12 "SANS II"** • Geometrical models • Contrast Variations • Time-resolved / stroboscopic • Applications **Andrew Jackson, ESS/LU**	
Fri 29 Oct	**L13 "INS I: Intro"** • Instrumentations (TAS/ToF) • Direct / Indirect geometry • Pulsed/Continuous • E/p conservation / k-space (reminder) • Examples (nuclear / magnetic) **Kim Lefmann, NBI**		Lunch	**L14 "INS II: Nuclear"** • Phonons (basics) • ω/τ domain • Cross sections • Applications **Gediminas Simutis, PSI**	**Ex. 10** • Simulation quiz: Ni single crystal in a Triple Axis Spectrometer • Quiz: Phonons of Ni **e-learning**
Sat 30 Oct	Free Weekend				
Sun 31 Oct	Free Weekend				

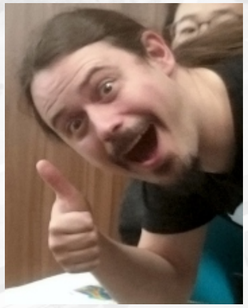
The School Program

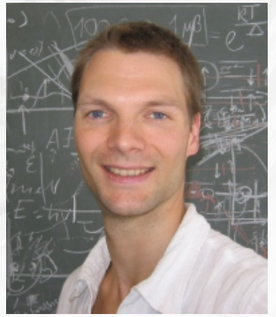
Week 3

Time / Date	Morning Session I 08:30 – 10:00	Morning Session II 10:30 – 12:00	12:00 - 14:00	Afternoon Session I 14:00 – 15:30	Afternoon Session I 16:00 – 17:30
Mon 1 Nov	**L15 "INS III: Magnetic"** • Spin waves • Magnetic Cross Section • Applications **Kim Lefmann, NBI**	**Ex. 11 Spin-waves** • Pen-and-paper problem **Kim Lefmann, NBI**	Lunch	Ex. 12: TUTORIAL - SpinW/OMDB • Modelling phonons/spin waves • Extract J's • Spin-W **Simon Ward, ESS/DMSC** **Johan Hellsvik, KTH**	Ex. 13: TUTORIAL - SpinW/OMDB • Modelling phonons/spin waves • Extract J's • Spin-W **Simon Ward, ESS/DMSC** **Johan Hellsvik, KTH**
Tue 2 Nov	*Help Session for Proposal Writing*	*Help Session for Proposal Writing*	Lunch	**L16 "QENS"** • Instrumentation • Energy-/timescales • Coherent / Incoherent • Diffusion, Molecular dynamics • Cross section &Isotope labeling **Aleksandar Matic, Chalmers**	
Wed 3 Nov	**L17 "Polarized Neutron Scattering"** • Polarizing/Flipping/Detecting the neutron spin (theory & technologies) • Basic theory • Examples (Elastic & Inelastic) **Werner Schweika, ESS**		Lunch	**L18 Keynote Lecture** *Societal Challenges* **"Sustainable Energy"** **Martin Månsson, KTH**	
Thu 4 Nov	**L19 Keynote Lecture** *Societal Challenges* **"Quantum Materials"** **Henrik Rønnow, EPFL**		Lunch	**L20 Keynote Lecture** *Societal Challenges* **"Engineering Materials/Processes"** **Richard Moat, OU**	*Help Session for Proposal Writing*
Fri 5 Nov	**L21 Keynote Lecture** *Societal Challenges* **"Life-Science"** **Jeremey Lakey, Newcastle University**		Lunch	**L22 Keynote Lecture** **"Future Science at ESS"** **Andreas Schreyer, ESS** Time: 15:00 – 16:30	**Closing Words** K. Lefmann, NBI M. Månsson, KTH
Sat 6 Nov	END OF SCHOOL				
Sun 7 Nov	END OF SCHOOL				

Your Teachers







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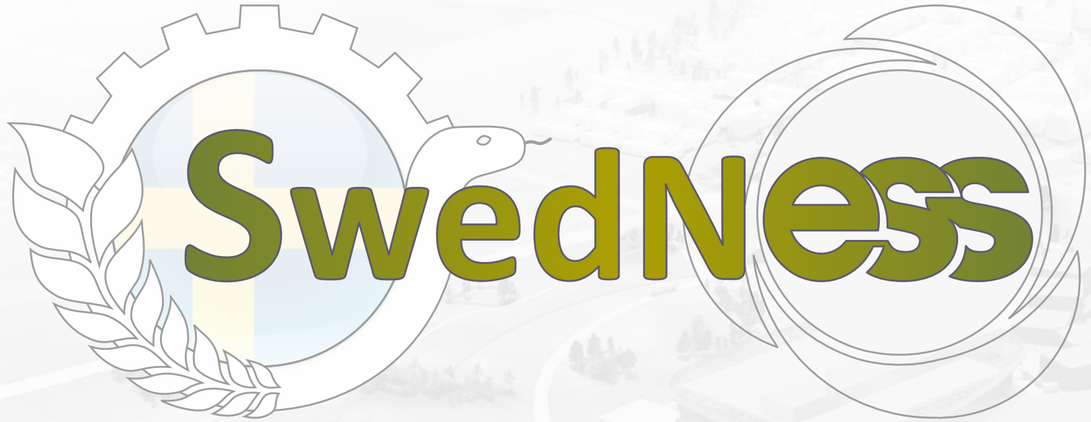

NNSP

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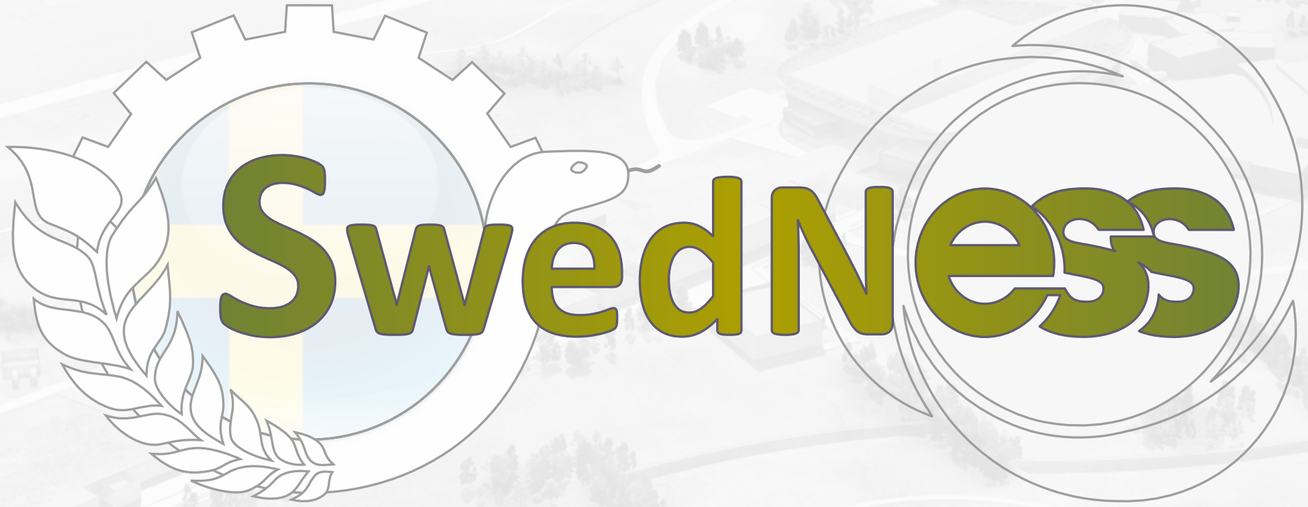
Swedish National Graduate School in Neutron Scattering



Swedish Neutron Education for Science & Society

Swedish Foundation for Strategic Research

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What is SwedNess?

- **Swedish national graduate school in neutron scattering that started officially in September 2016**

- **Collaboration between six Swedish universities with management at Uppsala 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.**

- **Total budget of 220 MSEK (~21 M€) running until 2026**

- **This allow us to fully fund course program as well as 40 PhD students with a individual budget of 4.5 MSEK each (salary + 200 kSEK/year in running budget per student)**

Intro Course in Neutron Scattering

- Theoretical part (lectures/exercises) is given together with the Nordic Neutron Science Program (NNSP) - Kim Lefmann.

- 2 weeks (4 ECTS) concertrated ”late summer” school in Tartu, Estonia

- Next Time: September 2022 (TBC)

- Funding for travel/hotel is available and the course is OPEN FOR EVERYONE !!!

- Fourth time we give this course

- So far ~150 students participated in this course (SE, DK, NO, Baltic states)

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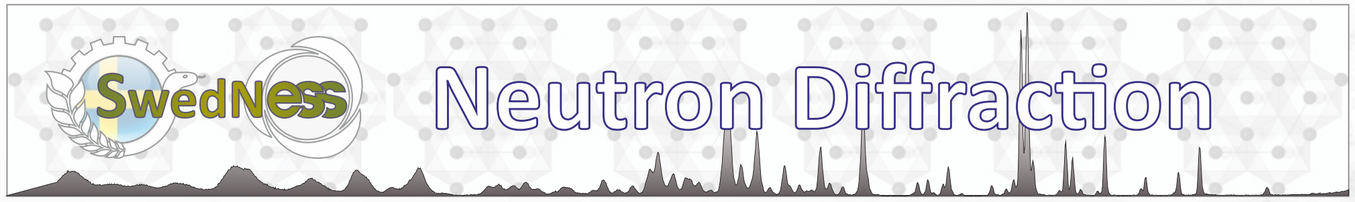
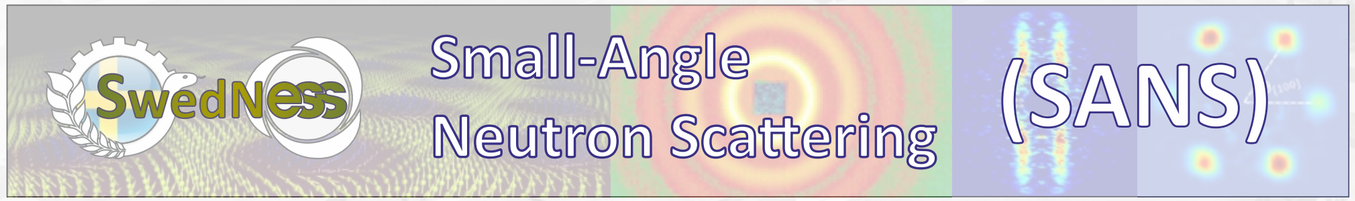
*Specialized Neutron Courses - **Techniques***



7.5 ECTS
Stockholm University

4 ECTS
Uppsala University



3 ECTS
Lund University

3 ECTS
Lund University

5 ECTS
Chalmers
ISIS

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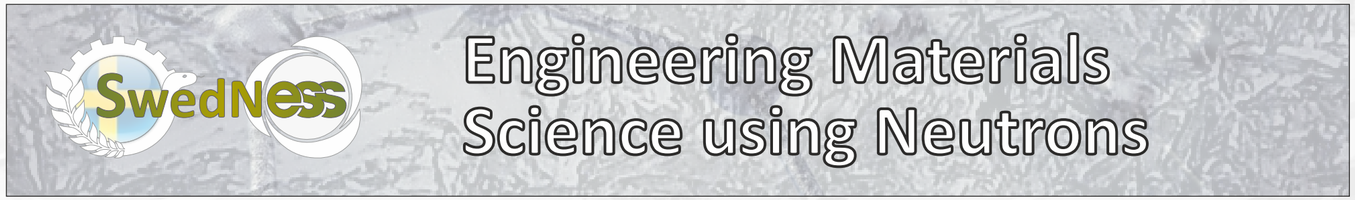
*Specialized Neutron Courses - **Topics***

5 ECTS
KTH
Uppsala University



5 ECTS
Linköping University,
Chalmers + KTH

5 ECTS
Linköping University

5 ECTS
KTH Royal Inst. Technology
NORDITA

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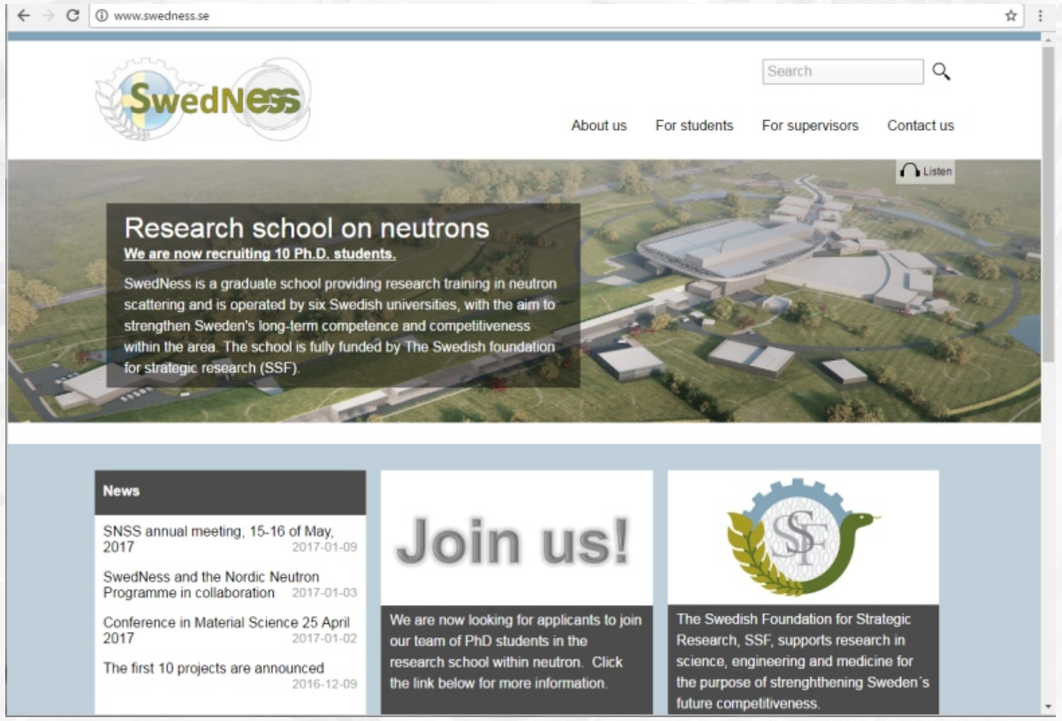
The SwedNess Course Catalogue

- **ALL courses, intro as well as specialized courses are aimed to be given annually!**
- **ALL courses are OPEN to EVERYONE (Universities outside SwedNess, industry...)**
- **ALL courses are FREE (except potential travel and accommodation in specialized courses)**
  (Covid-19 = online courses in progress)
- **Joint effort together with NNSP and e-neutrons.org**
- **Information is available at www.SwedNess.se**
- **So far we had close to 500 registered participants in our courses.**



RACIRI SUMMER SCHOOL

MIRAI 未来

- **SwedNess is also participating in & contributing to several other educational programs/efforts, e.g. RACIRI, MIRAI, etc.**

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Neutron Sources of the World

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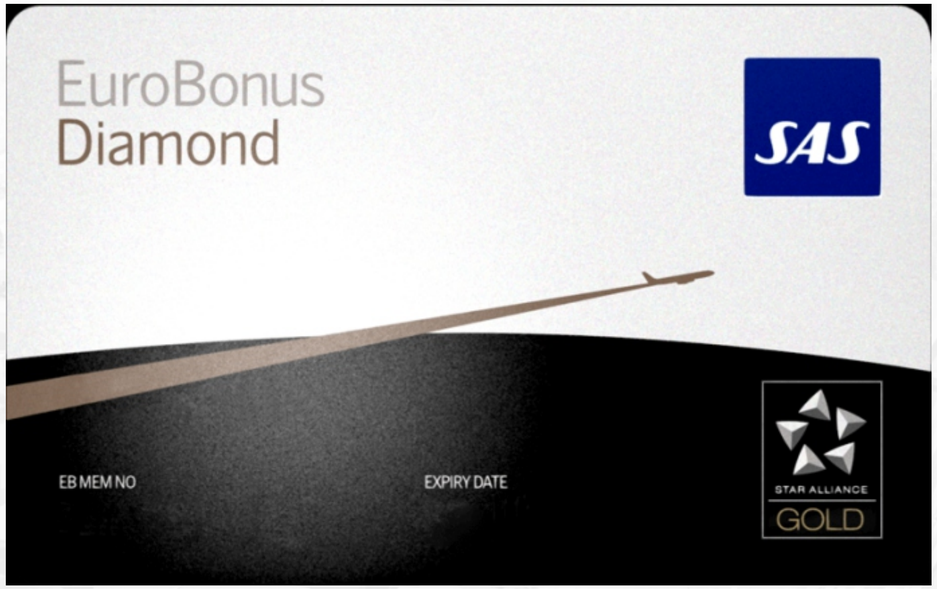
STAR ALLIANCE

GOLD



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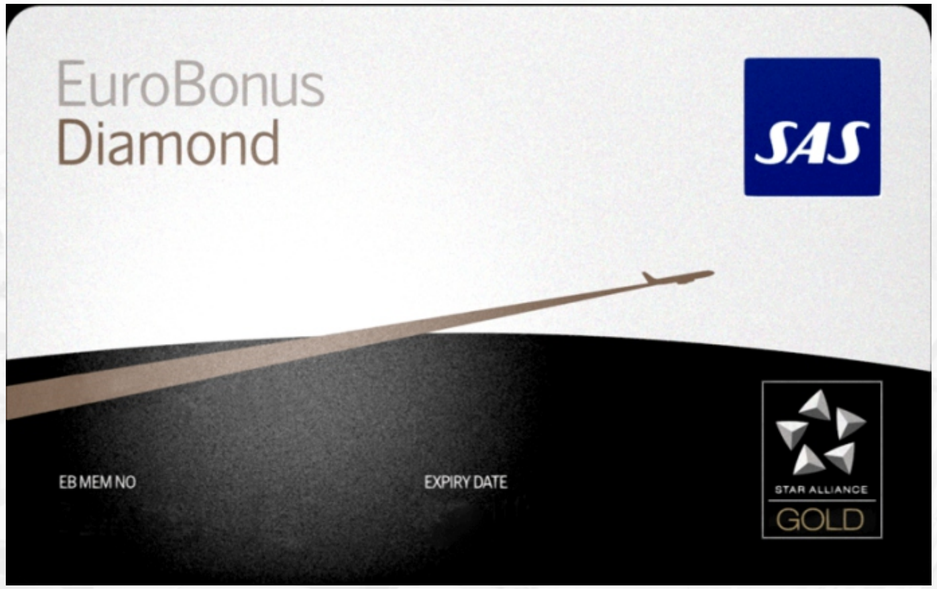
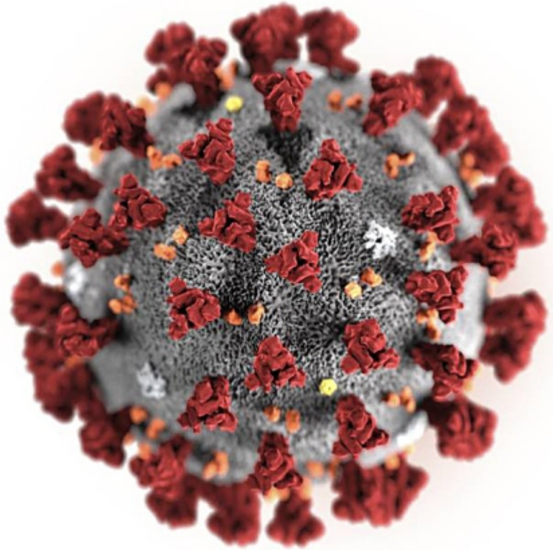
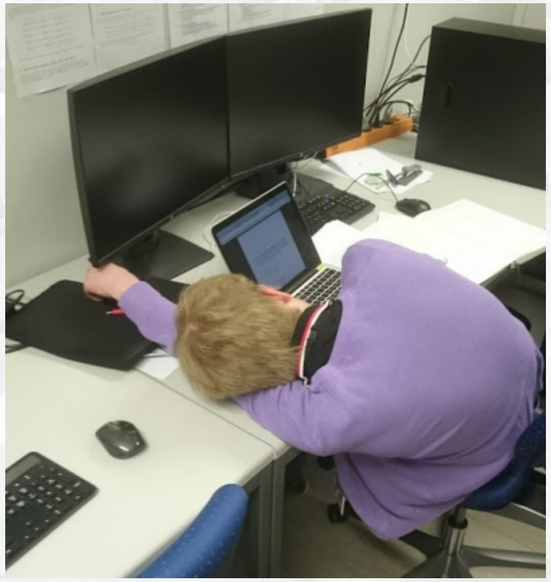
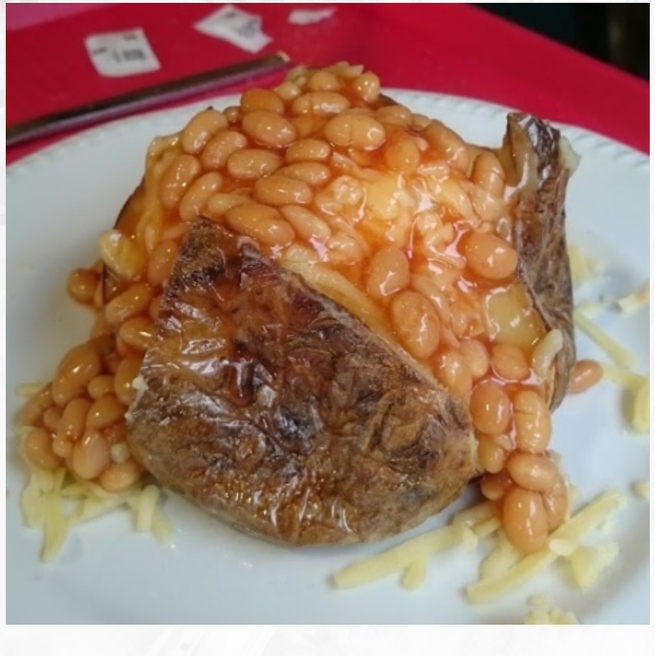
STAR ALLIANCE

GOLD









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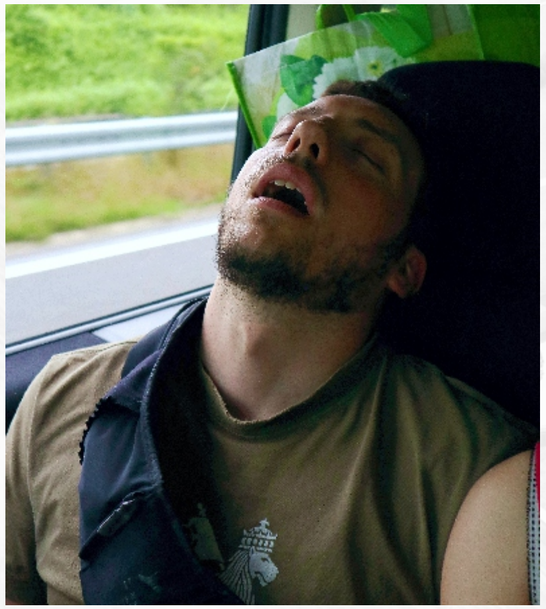

SUSTAINABLE MATERIALS & TECHNOLOGIES SMaRT RESEARCH

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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 (> 1 week 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.)
- If you plan to do experiments at different sources with same samples: consider
  activation of your samples (active sample transport is complicated and expensive!)
- Check necessary paperwork (visa!) at source and perform the mandatory ”safety training”

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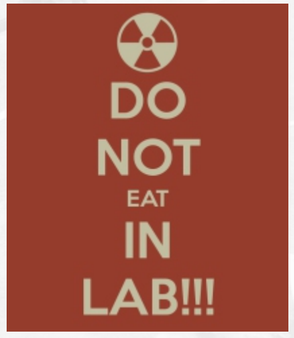
Paper Work / Administration / Safety

- 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.
- Nowadays: check also the rules for vaccine-pass etc.



Remember to apply for beamtime NOW !!!

NIST

DESY.

ISIS
Science & Technology
Facilities Council

SPring-8

OAK RIDGE
National Laboratory

TRIUMF

PAUL SCHERRER INSTITUT
PSI

SNS
SPALLATION NEUTRON SOURCE

diamond

MAX IV

ILL
NEUTRONS
FOR SCIENCE

ESRF
The European Synchrotron

J-PARC

ANSTO

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A Few Practical Things

- Lectures: conducted “live via zoom” except Kim’s afternoon lecture on 21 October (recording). We will record some lectures and make videos available (not all!). For lectures we wish to have questions via the zoom chat in order to keep a good flow and also to make video editing (for recorded lectures) easier. But do not hesitate to ask questions!!! Slides from the lectures will be made available.

- e-learning Exercises are conducted “on your own time” but during the dedicated sessions (in program) there will be online assistance via zoom (same link) available. ***Note the web-links in the program!***

- Web links: we have two parallel websites with the course material/info:

  https://indico.nbi.ku.dk/event/1670/

  https://www.neutrons.se/Tartu2021/

- Alumni Lectures from “old Tartu 2017 students” will be made available during these weeks as videos. Will both describe their projects and as well as give some “tips-and-tricks” for your conducting a PhD using neutrons. We advice to watch these towards the end of the school (or after).

- We have two more extensive Tutorials (Rietveld/Fullprof + SpinW/OMDB) that requires some preparations in the form of software installations. See the following slides...

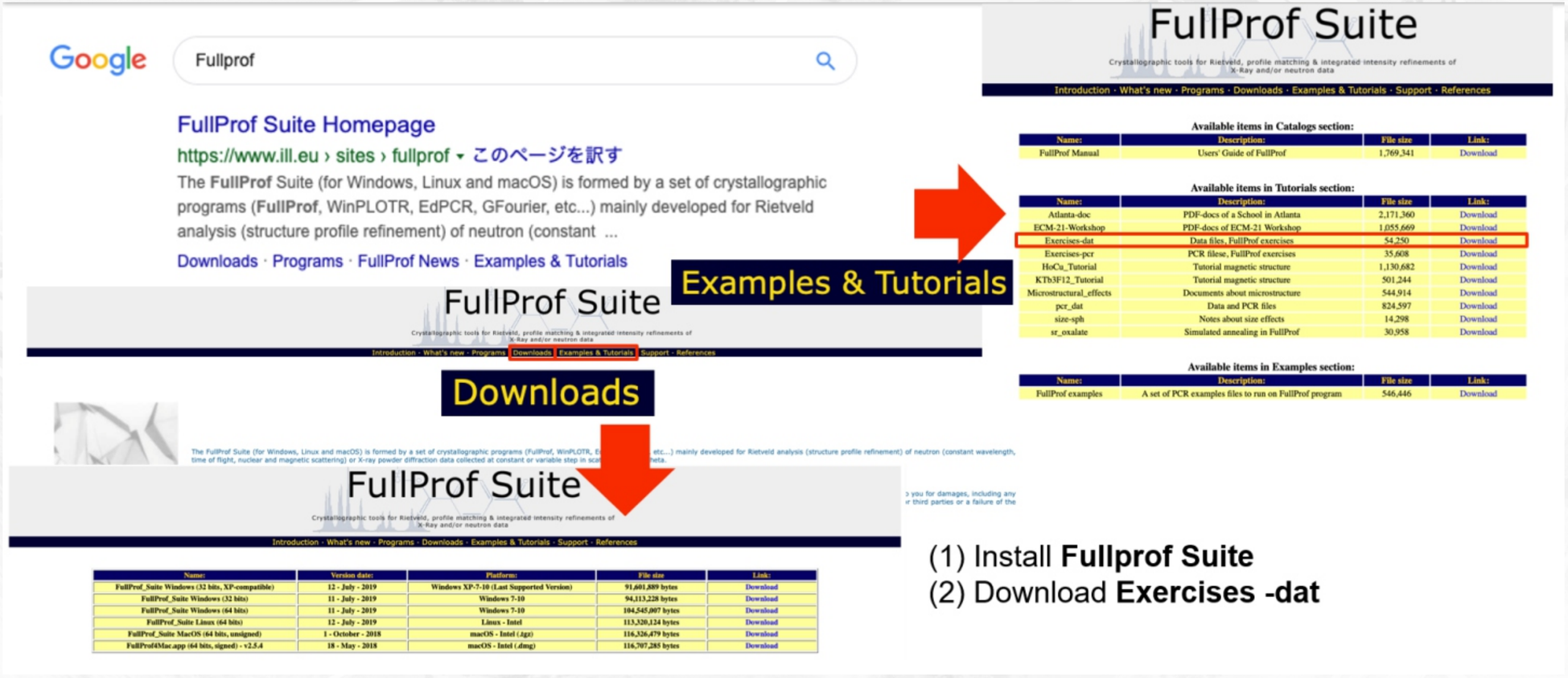
Diffraction / Fullprof & Vesta (26 October)

Please install the following (3) things during first week of the school:

1.

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

https://www.ill.eu/sites/fullprof/php/downloads.html

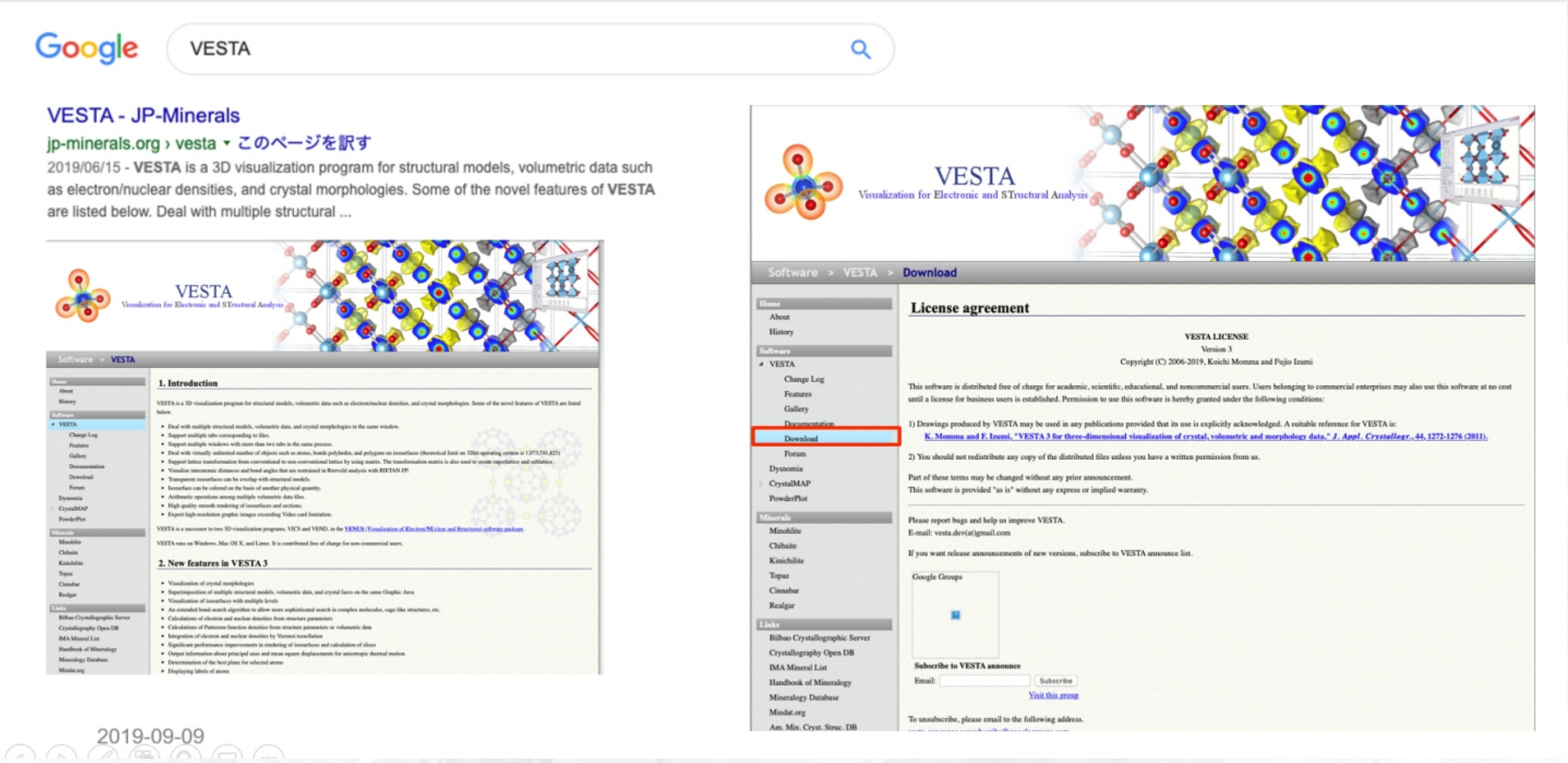


Diffraction / Fullprof & Vesta (26 October)

2.

Download / Install the Vesta software:

https://jp-minerals.org/vesta/en/download.html



3.

Have a “good” text editor installed on your laptop

Notepad++ : MS

TextWrangler: Mac

Modeling Magnetism / SpinW (1 November)

For the linear spin wave theory tutorial, a few software will be needed. Please try to complete the following preparations during the first week of the school and please ask if you need help!

(a) If you have access to a license, install Matlab. Many universities provide student licenses. If you do not want to (or can) install it on your computer you can also try the online version: **https://se.mathworks.com/products/matlab-online.html**

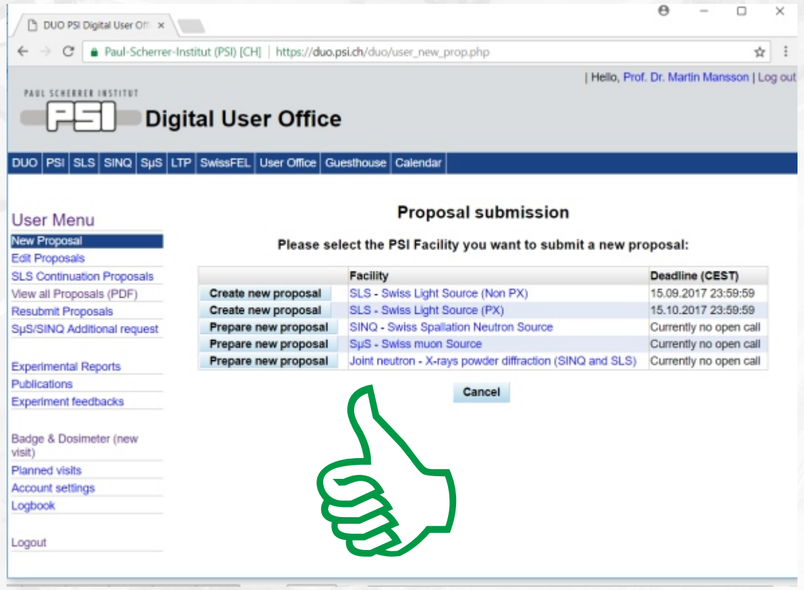
(b) Install the spinW software for linear spin wave theory from **https://github.com/spinw/spinw/releases/tag/v3.1**

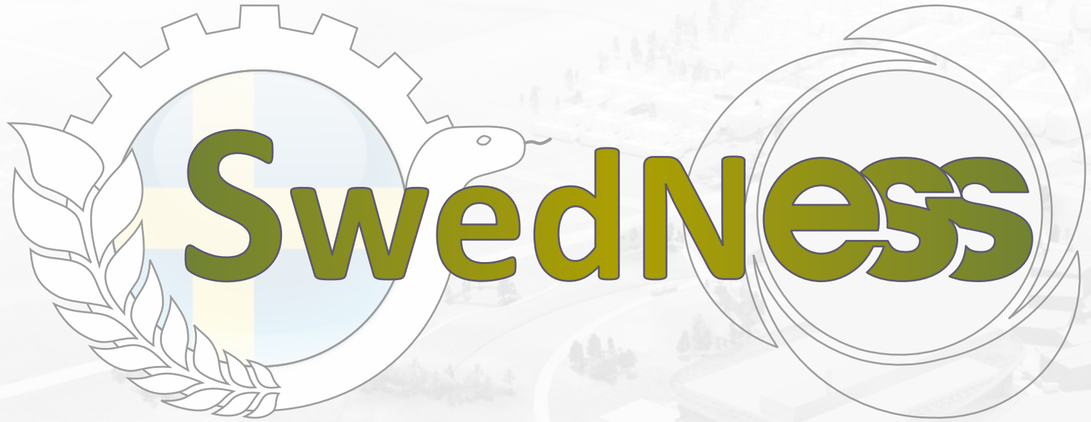
For the installation, additional details can be found at **http://spinw.org/installation/**

(c) Register for an account on the Organic Materials Database (OMDB) on **https://omdb.mathub.io/**

Examination of this Course (to obtain 4 ECTS)

- You should all write a proposal for neutron beamtime (details will follow...)
- Time during these 3 weeks and dedicated “assistance sessions”
- Submit to Me (Martin Månsson, condmat@kth.se) by latest 21 November 2021
- You also need to attend all/most lectures and actively conduct/participate in the e-learning exercises





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