



# Welcome to the NNSP/SwedNess Intro Course in Neutron Scattering











# Welcome to the NNSP/SwedNess Intro Course in Neutron Scattering











# Welcome to the NNSP/SwedNess Intro Course in Neutron Scattering













## 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?



 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.



1.843 billion €uro

0.7 billion €uro









1		7:00			12-20			17:20	10:00		
Application		-						-	-		
Sept   Figure   Foundation		8:30	14:00								
Solid   Foundation 1   Foundation 2   Foundation 3   Foundation 3   Foundation 4   Foundation 5   Foundation 6   Foundation	2 Sep	ARRIVAL DAY 1							*		
Foliable	2.0	Break-						Free	Dinner		
Mathematical   Mathematical   Foundation   Solid State Physics   Foundation   Solid	3 Sep				Lunch				*		
Foundation   Fou				-							
Series   S	12 18 18 18 18 18 18 18 18 18 18 18 18 18				Lunch	Foundation	Foundation	WELG	COME		
Welcome to the School   Production   Process   Lic Overview of the course   Production / Fifters / Detection   Production / Fifters / Detection / Production / Detection / Production / Production / Production / Detection / Production / Producti	4 Sep		Kim Lefmann,	Kim Lefmann,		Kim Lefmann,	Kim Lefmann,	RECE	PTION		
President   Practicals, Examination Process   Practicals, Examination Process   Production   Primitive / Safety at large-scale facilities   Elastic/helastic   Elas				ARRIVA	AL DAY 2	2					
Seep   Breat   Seep							L1.2: Intro				
Seep Breat Safety at large-scale facilities   Elastic/melastic   Elast			The state of the s		Lunch		0-4-3-6-4000				
Seep   Nation Memory   Seep   Nation   Seep   Nation Memory   Seep	5 Son	Break-						Free			
Martin Mânsson, KTH   Martin Mânsson, KTH   Kim Lefmann, University of Copenhagen   Martin Mânsson, KTH	ээср	fast	Safety at large-scale facilities	·		_	Conferency inconference	Time	*		
12: Neutron Sources & Instrumentation			Kim Lefmann, University of Copenhagen	·							
Sources Moderators   - Monchromators / choppers   - Outz: Test your knowledge of neutron electron   - Outz: Test your knowledge of neutron of protection   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Magnetism   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron   - Outz: Test your knowledge of neutron sources and instrumentation   - Outz: Test your knowledge of neutron sources and instrumentation   - Outzer test your knowledge of neutron sources and instrumentation   - Outzer test your knowledge of neutron sources and multimentation   - Outzer test your knowledge of neutron sources and instrumentation   - Outzer test your knowledge of neutron			-	·							
Sop   Freal							Ex. 2				
Collimation / Filters / Guides   Outr Test your knowledge of neutron sources and instrumentation   Celearning							Ouiz: The neutron cross section				
Potential Potent	6 Sep				Lunch	·					
Kim Lefmann, University of Copenhagen   Catch up on assignments/e-learning and inquire about things you did not understand   Scriptallography   Crystallography   Crystallog		fast					• •		Time		
Late Magnetic Scattering   Magnetism   Nuclear/Magnetic Scattering   Nuclear/Magnetic Scattering   Catch up on assignments/e-learning and inquire about things you did not understand   Late Magnetism   Nuclear/Magnetic Scattering   Nuclear/Magnetic Scattering   Catch up on assignments/e-learning and inquire about things you did not understand   Late Magnetism   Nuclear/Magnetic Scattering   Nuclear/Magnetic Scattering   Late Magnetism   Nuclear/Magnetic Scattering   Nu							(e-learning)				
## Agnetism    Nuclear/Magnetic Scattering   Catch up on assignments/e-learning and inquire about things you did not understand   Lunch   Simulation quiz: Diffraction from powder				(e-learning)			For 2 #Designment letting of Nill				
** Nuclear/Magnetic Scattering Catch up on assignments/e-learning and inquire about things you did not understand Underst			_	inquire about things you did not understand  Lunch		Ex. 5 Reciprocal lattice of Ni					
Sep   Freak feat   Fast   Fa			_		Lunch		Quiz: Reciprocal lattice of Ni		Dinner		
Kim Lefmann, University of Copenhagen   Johan Cedervall, Stockholm Univ.   (e-learning)	7 Sep					Brillouin Zone					
L6: Diffraction   L7: Diffraction   L7: Diffraction   Ex. 5			Kim Lefmann Halvareity of Cononbagon			takan Gadamatti Shadhalar Hair	powder				
Sep   Break-fast   L6: Diffraction I			Kim Leimann, University of Copennagen			Johan Cedervall, Stockholm Univ.	(e-learning)				
* Intro * Neutrons vs. X-rays * Intro * Neutrons vs. X-rays * Page 1  * Intro * Neutrons vs. X-rays * Intro * Neutrons vs. X-rays * Page 2  * Intro * Neutrons vs. X-rays * Page 2  * Intro * Neutrons vs. X-rays * Page 2  * Intro * Neutrons vs. X-rays * Page 2  * Intro * Neutrons vs. X-rays * Page 2  * Intro * Neutrons vs. X-rays * Page 2  * Wiki problem: Bragg scattering from non-Bravals lattices * Wiki problem: Bragg scattering from non-Bravals lattices * Dinner * Neutrons vs. X-rays * Wiki problem: Bragg scattering from non-Bravals lattices * Dinner * In plane / out of plane * In plane / out of plane * Applications * Adrian Rennie, Uppsala University * Page 2  * Page 2  * Page 2  * Wiki problem: Bragg scattering from non-Bravals lattices * Dinner * Adrian Rennie, Uppsala University * Dinner * GALA DINNER * GALA DINNER * GALA DINNER * Dinner * The Rietveld method * Fullprof intro + start of refinement * When is Xray or Neutron diffraction suitable? * Wiki problem: Bragg scattering from non-Bravals lattices * Dinner New 2  * Dinner * GALA DINNER * GALA DINNER * Dinner * GALA DINNER * D			L6: Diffraction I	L7: Diffraction II		Ex. 4 - TUTORIAL					
** Neutrons vs. X-rays  ** Total Scattering  ** Etc.  ** Unch  ** Fullprof intro + start of refinement  ** When is Xray or Neutron diffraction  ** suitable?  ** Wiki problem: Bragg scattering from  non-Bravais lattices  ** Johan Cedervall, Stockholm Univ.  ** Johan Cedervall, Stockholm Univ.  ** Distorted Born approximation  ** Specular/off-specular  ** Optical Matrix  ** Optical Matrix  ** Optical Matrix  ** Catch up on assignments/e-learning and inquire about things you did not understand  ** Free Time  ** Applications  ** Adrian Rennie, Uppsala University  ** Distorted Born approximation  ** In plane / out of plane  ** Applications  ** Adrian Rennie, Uppsala University  ** Dinner  ** Optical Matrix  ** Adrian Rennie, Uppsala University  ** Optical Matrix  ** Adrian Rennie, Uppsala University  ** Optical Matrix  ** Distorted Born approximation  ** Applications  ** Applications  ** Adrian Rennie, Uppsala University  ** Optical Matrix  **						The Birth old on the d	Fullprof refinement continued				
Break- fast  Johan Cedervall, Stockholm Univ.  L8: Reflectometry I  Instrumentation/applications  Specular/off-specular  Optical Matrix  Optical Matrix  Kinematic Approximation  Adrian Rennie, Uppsala University  Let.  L9: Reflectometry II + GiSANS  Distorted Born approximation  GiSANS Instrumentation  In plane / out of plane  Applications  Adrian Rennie, Uppsala University  Dinner  Catch up on assignments/e-learning and inquire about things you did not understand inquire about things you did							Lunch		When is Xray or Neutron diffraction		Dianas
Johan Cedervall, Stockholm Univ.  L8: Reflectometry I  In Instrumentation/applications Specular/off-specular Optical Matrix Kinematic Approximation Adrian Rennie, Uppsala University  Johan Cedervall, Stockholm Univ.  L8: Reflectometry II + GiSANS Instrumentation Specular/off-specular Adrian Rennie, Uppsala University  L8: Reflectometry II + GiSANS Instrumentation In plane / out of plane Adrian Rennie, Uppsala University  Adrian Rennie, Uppsala University  Optical Matrix Adrian Rennie, Uppsala University  Dinner	8 Sep		- Weddolls vs. X-rays	_				Talipior intro i start of remement			
Johan Cedervall, Stockholm Univ.  L8: Reflectometry I  Instrumentation/applications  Specular/off-specular Optical Matrix Kinematic Approximation Adrian Rennie, Uppsala University  L8: Reflectometry I  Simulation quiz: Reflectometer  In plane / out of plane Adrian Rennie, Uppsala University  Adrian Rennie, Uppsala University  Dinner  Dinner											
See Break-  L8: Reflectometry I  Instrumentation/applications Specular/off-specular Optical Matrix Kinematic Approximation Adrian Rennie, Uppsala University  L9: Reflectometry II + GiSANS Distorted Born approximation GiSANS Instrumentation In plane / out of plane Adrian Rennie, Uppsala University  L9: Reflectometry II + GiSANS Distorted Born approximation GiSANS Instrumentation In plane / out of plane Applications Adrian Rennie, Uppsala University  Dinner  Dinner			Johan Cedervall, Stockholm Univ.	Johan Cedervall, Stockholm Univ.				John Codernell Standbales Heis	non-Bravais lattices		
• Instrumentation/applications • Specular/off-specular • Optical Matrix • Kinematic Approximation  Adrian Rennie, Uppsala University  • Instrumentation/applications • Simulation quiz: Reflectometer • Optical Matrix • In plane / out of plane • Applications  Adrian Rennie, Uppsala University  • Distorted Born approximation • GiSANS Instrumentation • In plane / out of plane • Applications  Adrian Rennie, Uppsala University  • Dinner • Dinner								Jonan Cedervall, Stockholm Univ.	Johan Cedervall, Stockholm Univ.		
• Specular/off-specular • Optical Matrix • Kinematic Approximation Adrian Rennie, Uppsala University  • Specular/off-specular • Optical Matrix • Kinematic Approximation Adrian Rennie, Uppsala University  • Simulation quiz: Reflectometer • In plane / out of plane • Applications  Adrian Rennie, Uppsala University  • GALA DIN-NER  GALA DIN-NER  Dinner				Ex. 6		-					
Optical Matrix     Kinematic Approximation     Adrian Rennie, Uppsala University  Optical Matrix     Kinematic Approximation     Adrian Rennie, Uppsala University  In plane / out of plane     Applications  Adrian Rennie, Uppsala University  DINNER  DINNER  DINNER  Dinner				e content of the cont			Cotch up on assignments to termine and		DIN-		
Kinematic Approximation     Adrian Rennie, Uppsala University      Break-    Break-   FREE DAY / EXCURSION      Applications   Adrian Rennie, Uppsala University	9 Sep			Simulation quiz: Reflectometer							
Adrian Rennie, Uppsala University  Adrian Rennie, Uppsala University  Dinner			·	(e-learning)			mane about things you did not understand	Time			
10 Break- Properties FREE DAY / EXCURSION Dinner											
FREE DAY / EXCURSION			Adrian Kennie, Oppsala University			Adrian Kennie, Oppsala University			D.		
Sep 10.5				FR	EE DAY	/ EXCURSION					
	Sep	1031									



## **The School Program**



					. 470 1 1			
11 Sep	Break- fast	L10: Neutron Imaging	Simulation quiz: Bragg Edge Imaging on Viking Sword  (e-learning)	Lunch	L11: SANS I  Instrumentation2 Scattering Length Density Form-/Structure Factor Approximations  Andrew Jackson, Lund University / ESS	Simulation quiz: Small Angle     Neutron Scattering     Resolution (wavelength vs. angle)     Data Treatment  (e-learning)	Free Time	Dinner *
12 Sep	Break- fast	Geometrical models     Contrast Variations     Time-resolved / stroboscopic     Applications  Andrew Jackson, Lund University / ESS	Catch up on assignments/e-learning and inquire about things you did not understand	Lunch	L13: INS I "Intro"  Instrumentations (TAS/ToF)  Direct / Indirect geometry  Pulsed/Continuous  E/p conservation  k-space (reminder)  Examples (nuclear / magnetic)  Kim Lefmann, University of Copenhagen	Ex. 9  Simulation quiz: Ni single crystal in a Triple Axis Spectrometer Quiz: Phonons of Ni  (e-learning)	Free Time	Dinner *
13 Sep	Break- fast	L14: INS II "Nuclear"  Phonons (basics)  ω/τ domain  Cross sections  Applications  Gediminas Simutis, Paul Scherrer Institute	L15: INS III "Magnetic"	Lunch	Ex. 10 - TUTORIAL  Modelling phonons/spin waves Extract J's Spin-W  Simon Ward, ESS / DMSC	Modelling phonons/spin waves     Extract J's     Spin-W  Simon Ward, ESS / DMSC	Free Time	Dinner *
14 Sep	Break- fast	Polarized Neutron Scattering: BASICS     Polarizing/Flipping/Detecting the neutron spin (theory & technologies)     Basic theory     Examples (Elastic & Inelastic)  Werner Schweika, ESS	L17: QENS  Instrumentation Energy/time-scales Coherent / Incoherent Diffusion, Molecular dynamics Cross section &Isotope labeling  Mark Telling, STFC/ISIS	Lunch	Ex. 11 - TUTORIAL  Polymer Dynamics (dynamics / diffusion) Isotope labeling  Mark Telling, STFC/ISIS Miriam Koppel, Univ. Tartu	Ex. 11 (continued)  Polymer Dynamics (dynamics / diffusion) Isotope labeling  Mark Telling, STFC/ISIS Miriam Koppel, Univ. Tartu	Free Time	Dinner *
15 Sep	Break- fast	L18: Keynote Lecture: "Challenge 1"  Neutrons for Sustainability  Martin Månsson  KTH Royal Institute of Technology  Sweden	L19: <u>Keynote Lecture</u> : "Challenge 2"  Neutrons for Life  Trevor Forsyth  LINXS, Sweden	Lunch	L20: <u>Keynote Lecture</u> : "Challenge 3"  Neutrons for "Skyrmions"  Henrik Rønnow  EPF Lausanne, Switzerland	L21: Keynote Lecture: "Challenge 4"  Neutrons for Engineering  Richard Moat  Open University, UK	Free Time	End Din- ner
16 Sep	Break- fast	Help for Proposal Writing  +  Visit of ESS site		Lunch	L22: <u>Key-Note Lecture</u> : "ESS"  Future Science at ESS  Andreas Schreyer, ESS	Help for Proposal Writing + Visit of ESS site		Dinner *
17 Sep	Break- fast	DEPARTURE DAY						

<sup>\*</sup> Dinners during the normal lecture days are your own responsibility. SwedNess/NNSP are only organizing the "Welcome Reception", "Gala Dinner" and "End Dinner". Lunch is included.

Most of the exercises (Ex.) are conducted individually via our e-learning platform ( https://pan-learning.org/)

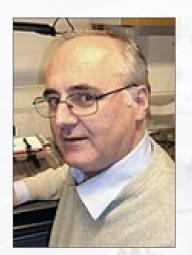


# **Your Teachers**



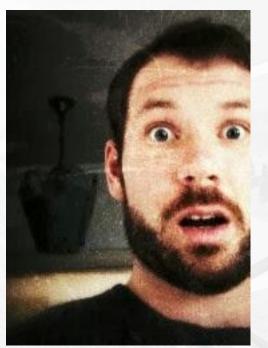






























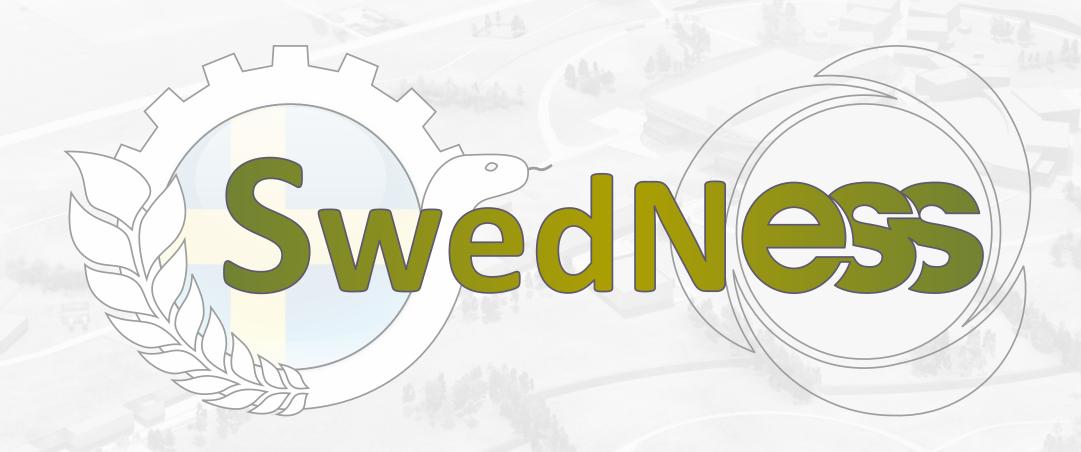




# 

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

# Swedish National Graduate School in Neutron Scattering



Swedish Neutron Education for Science & Society



#### 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:

#### **CHALMERS**











Swedish Foundation for

Strategic Research



- Fully funded by the <u>Swedish Foundation for Strategic Research</u> (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 \ \S\P

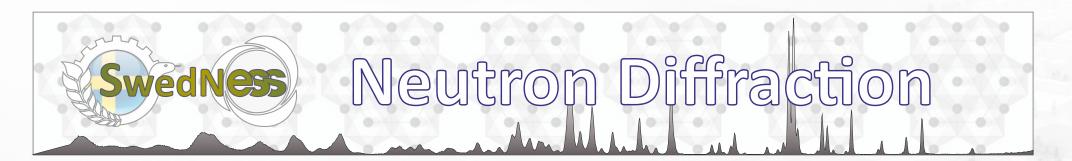


- Theoretical part (lectures/exercises) is given together with the Nordic Neutron Science Program (NNSP) - Kim Lefmann.
- 2 weeks (4 ECTS) concertrated "late summer" school (now @ESS with visit of the facility)
- Next Time: September 2023 (TBC)
- Funding for travel/hotel is available and the course is **OPEN FOR EVERYONE!!!**
- Fifth time we give this course
- So far ~200 students participated in this course (SE, DK, NO, Baltic states)





#### Specialized Neutron Courses - Techniques



**7.5 ECTS Stockholm University** 



4 ECTS **Uppsala University** 



3 ECTS **Lund University** 



3 ECTS **Lund University** 

Neutron Spectroscopy **SwedNess** 

**5 ECTS Chalmers** ISIS

#### Specialized Neutron Courses - Topics



Neutrons for the study of electrochemical processes



Engineering Materials
Science using Neutrons

Swedness

Neutrons for Life Science



Neutrons & Muons for Magnetism

5 ECTS
KTH
Uppsala University

5 ECTS
Linköping University,
Chalmers + KTH

5 ECTS
Linköping University

5 ECTS
KTH Royal Inst. Technology
NORDITA

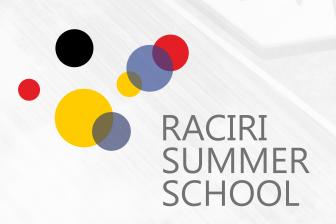
#### The SwedNess Course Catalogue



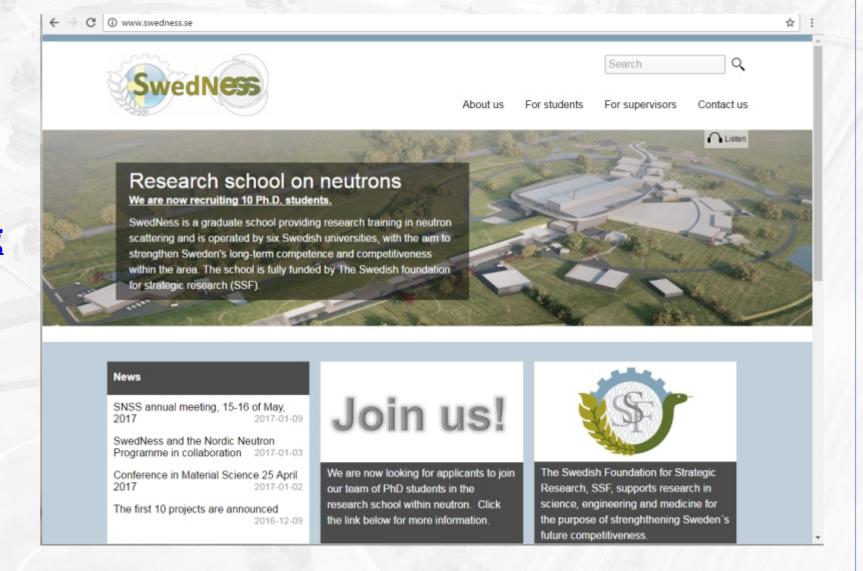
- ALL courses, intro as well as specialized courses are aimed to be given annually!
- ALL courses are OPEN to EVERYONE (Universities outside SwedNess, industry...)
- ALL courses are FREE (except potential travel and accommodation in specialized courses)

(Covid-19 = online courses in progress)

- Joint effort together with NNSP and pan-learning.org
- Information is available at www.SwedNess.se
- So far we had close to 500 registered participants in our courses.







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



## **Neutron Sources of the World**







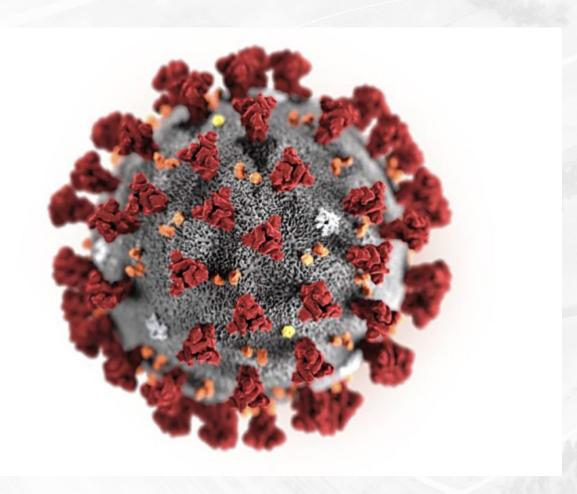


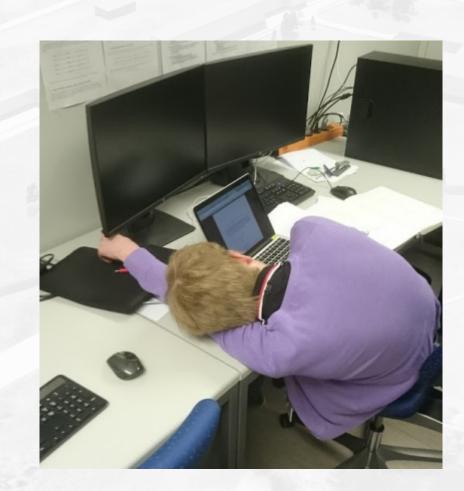




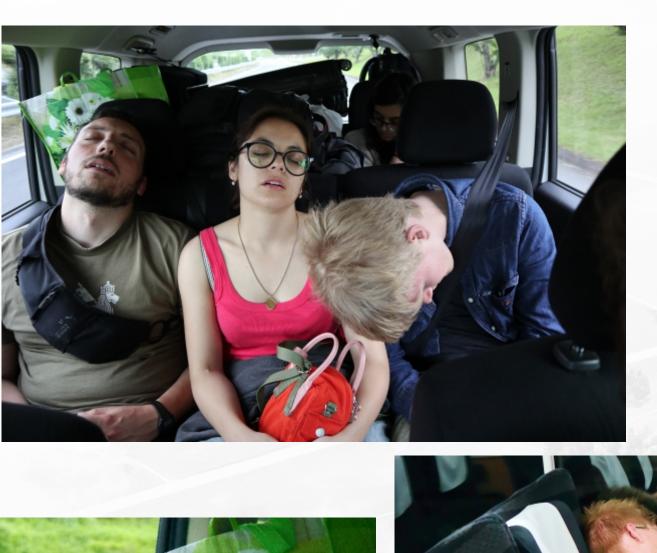




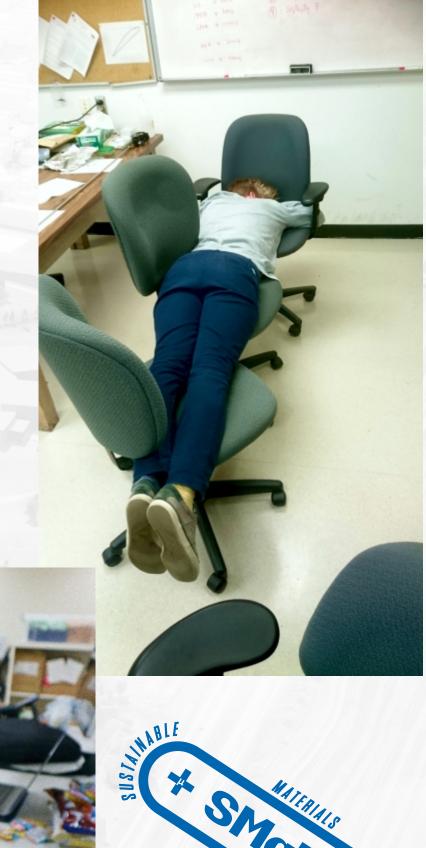
















## Prepare for Beamtime = Proposal Writing



- Idea for how neutrons can help your research (specific question = piece of the puzzle)
- O Talk to an expert (this will soon be You !!!)
- O Consider your sample!!! (available size/mass, crystal/powder/thin film).
- Think about if you sample contains elements with low scattering or high absorption <a href="http://www.ncnr.nist.gov/resources/n-lengths/">http://www.ncnr.nist.gov/resources/n-lengths/</a>
- O Select appropriate source & instrument for your experiment (<a href="check deadlines + shutdowns!">check deadlines + shutdowns!</a>)
- O 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
- O Cross your fingers and wait for the review committee + in some cases "national quota"
- O 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"



# 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!!!







ISIS
Science & Technology
Facilities Council

















The European Synchrotron







### A Few Practical Things



- Slides from the lectures will be made available (as soon as possible but sometimes "a bit later").
- e-learning Exercises are conducted "individually" during the dedicated sessions (in program) and there
  will be assistance available. Note the web-links in the program (PDF file)!
- Web links: we have two parallel websites with the course material/info:

https://indico.nbi.ku.dk/event/1828/

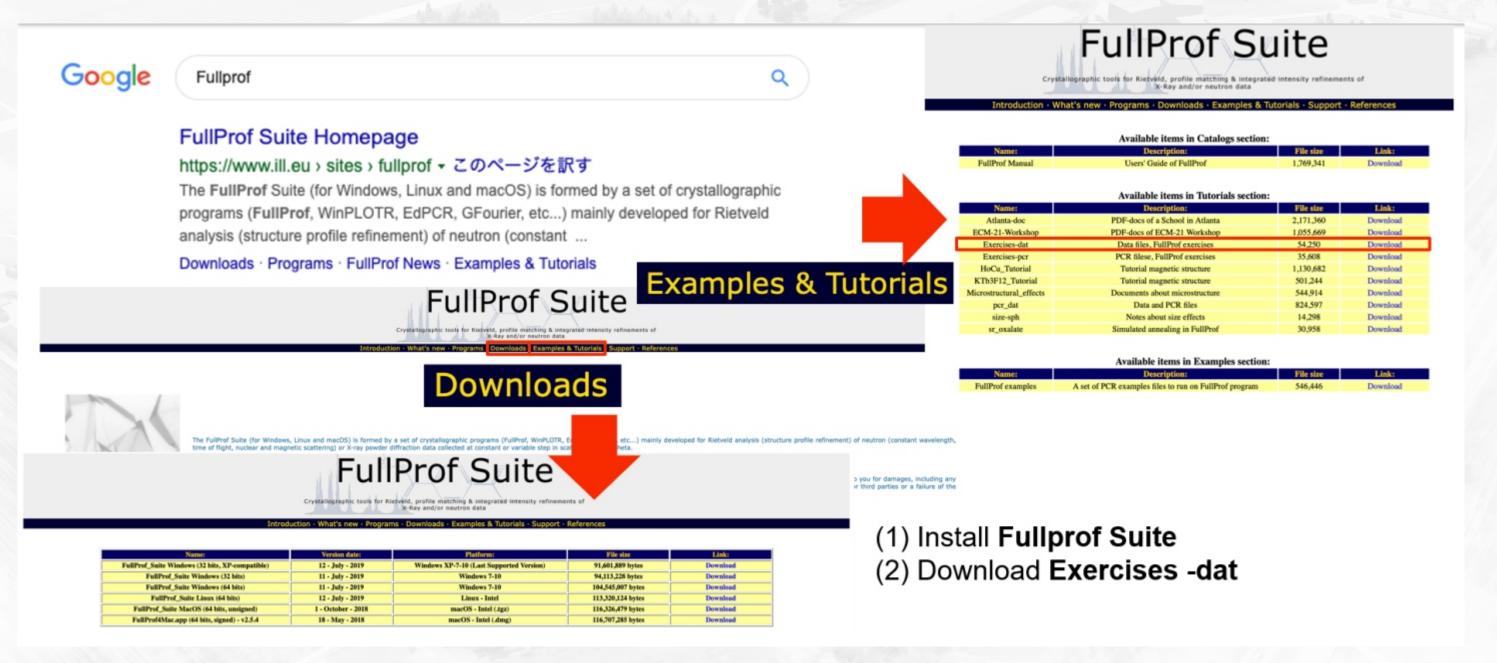
https://www.neutrons.se/Tartu2022/

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

# Diffraction / Fullprof & Vesta (8 September)

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

Download / Install the Fullprof suite + Exercises-dat (tutorials) https://www.ill.eu/sites/fullprof/php/downloads.html



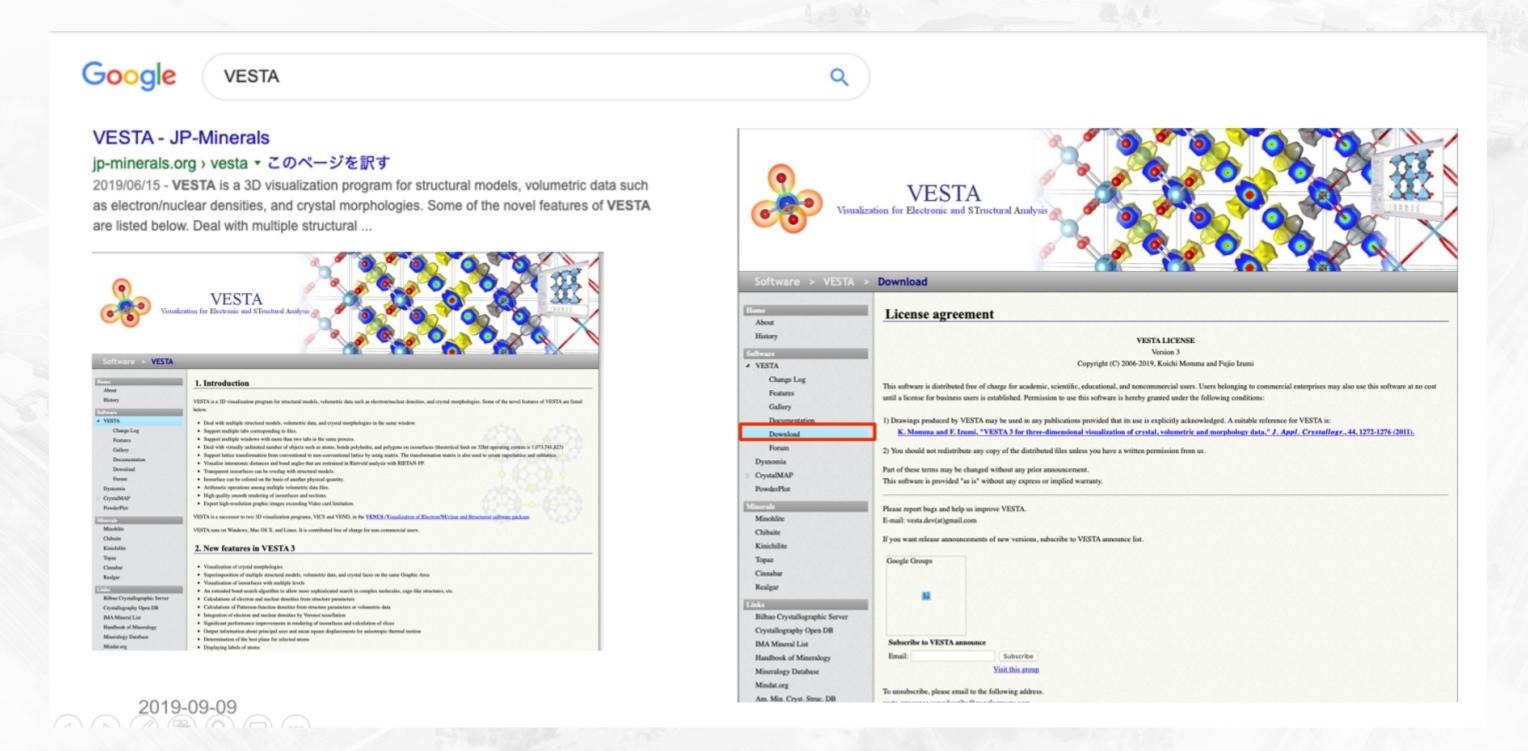


# Diffraction / Fullprof & Vesta (8 September)



2.

Download / Install the Vesta software: <a href="https://jp-minerals.org/vesta/en/download.html">https://jp-minerals.org/vesta/en/download.html</a>



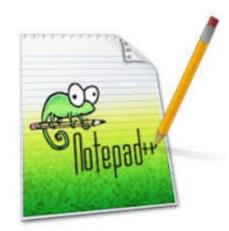


# Diffraction / Fullprof & Vesta (8 September)



3.

Have a "good" text editor installed on your laptop



Notepad++: MS



TextWrangler: Mac





# Modeling Magnetism / SpinW (13 September)



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: <a href="https://se.mathworks.com/products/matlab-online.html">https://se.mathworks.com/products/matlab-online.html</a>
- (b) Install the spinW software for linear spin wave theory from <a href="https://github.com/spinw/spinw/releases/tag/v3.1">https://github.com/spinw/spinw/releases/tag/v3.1</a>
  - For the installation, additional details can be found at <a href="http://spinw.org/installation/">http://spinw.org/installation/</a>
- (c) Register for an account on the Organic Materials Database (OMDB) on <a href="https://omdb.mathub.io/">https://omdb.mathub.io/</a>

## Quasi-Elastic Neutron Scattering (QENS) / Mantid

For QENS Lecture / Exercise Wednesday 14 September Please download and install the latest version of Mantid 4.0.0





https://sourceforge.net/projects/mantid/files/4.0/mantid-4.0.0-win64.exe/download

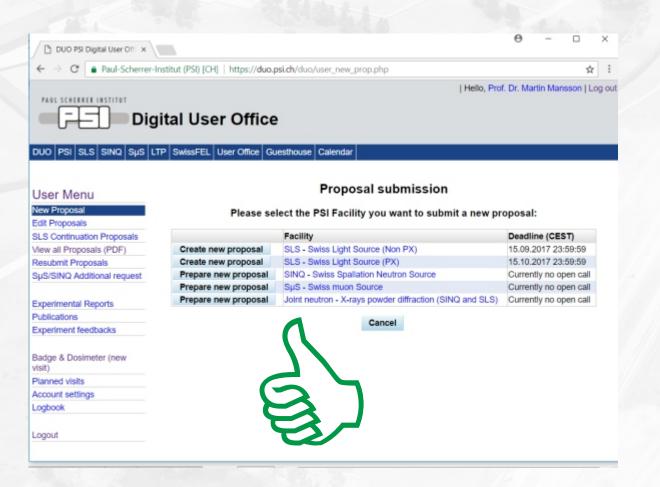


## Examination of this Course (to obtain 4 ECTS)



- You should all write a proposal for neutron beamtime (details will follow...)
- Time during these 2 weeks and dedicated "assistance sessions"
- Submit to Me (Martin Månsson, condmat@kth.se) by latest 30 September 2022 at 23:59
- You also need to attend all/most lectures and actively participate in the e-learning exercises









# 

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