



# ISIS Reflectivity Training Course

16<sup>th</sup> to 25<sup>th</sup> November 2021

## COURSE INSTRUCTIONS

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## 2 GENERAL NOTES

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Dear course participant,

Welcome to the first ISIS Virtual Reflectometry Training course! We'd like to give you an idea of what you can expect and what we hope to achieve over the four course days. The course is designed to give you a comprehensive overview over the technique of reflectometry, starting from first principles and theoretical background and finishing with hands-on data analysis. By the end of the course you should be able to design and run a successful reflectivity experiment and then analyse your data for publication.

You can find the latest timetable, course materials and Zoom links here:

<https://indico.stfc.ac.uk/event/355/timetable/?layout=room#20211116.detailed>

As this is a fully remote course, we rely on several different online environments (Zoom, Slack, IDaaS), which opens the possibility of technical problems. For the smooth running and enjoyment of the course, we'd like to ask you to check all the relevant environments, as detailed below. You will also need to make sure that you have the following apps (ideally latest versions) installed on your Laptop/PC/mobile:

- Zoom (<https://zoom.us/>)
- Slack (<https://slack.com/intl/en-gb/>)

You should not need to install any other software, but you will require access to the ISIS data analysis environment, as described in the following sections.

We would advise you to attend the course using a device with a large screen or ideally two screens. Don't worry if you are not able to, you will still be able to attend, but it will involve more scrolling and switching windows.

The timetable structure alternates lectures with demonstrations and practicals. We would like to encourage you to participate actively, ask questions and explore all available resources. We will use Slack as tool for written communication, in parallel with the Zoom sessions. That way, you will be able to communicate with the other course participants and the lecturers. You can ask questions and exchange ideas.

In order to get the most out of the course, it is important that you familiarise yourself with the course content as much as possible, which will be available ahead of the course and after the course has finished. Please take the time to learn about the principles of neutron facilities and neutron scattering in general by visiting for instance the ISIS website. Here is a minimal checklist:

|                          |  |
|--------------------------|--|
| <input type="checkbox"/> | Zoom installed   |
| <input type="checkbox"/> | Slack installed (join <a href="#">ISIS Reflectivity Course</a> )                           |
| <input type="checkbox"/> | ISIS User Office Registration (Section 3)  |
| <input type="checkbox"/> | IDaaS access (Section 4)   |
| <input type="checkbox"/> | In IDaaS, open Applications->Examples->NTC 2021 Course Material and copy folder to Desktop |
| <input type="checkbox"/> | Submit own problem (optional, see Section 6)   |

If you encounter any problems, please don't hesitate to contact the course organisers [maximilian.skoda@stfc.ac.uk](mailto:maximilian.skoda@stfc.ac.uk) or [luke.clifton@stfc.ac.uk](mailto:luke.clifton@stfc.ac.uk).

We are looking forward to meeting you soon and we hope you will enjoy the course!

Best wishes,

Max and Luke

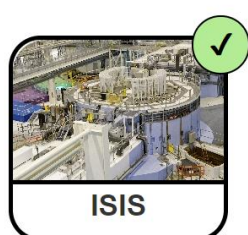
### 3 ISIS USER OFFICE REGISTRATION

In order to access the main data analysis and training environment (IDAaaS), it is necessary to create and account with the ISIS user office. Navigate to

<https://users.facilities.rl.ac.uk/auth/CreateAccount.aspx>

Fill in your details and register for the ISIS facility:

Please select all the facilities you wish to register with:



### 4 IDAAS CHECK

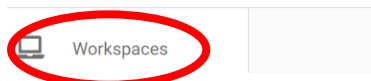
Approximately 10 minutes after the user office registration, you should be able to access the “ISIS Data Analysis as a Service” (IDAaaS) website:

<https://isis.analysis.stfc.ac.uk/>

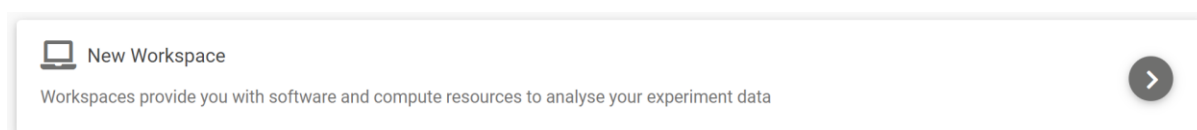
Please familiarise yourself with the data analysis environment and read the help topics.

From the left hand list of options, select

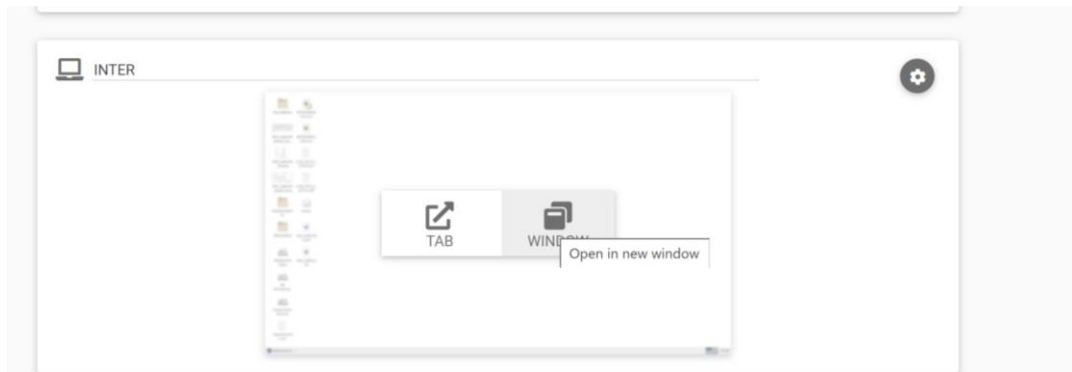
 ISIS Data Analysis as a Service



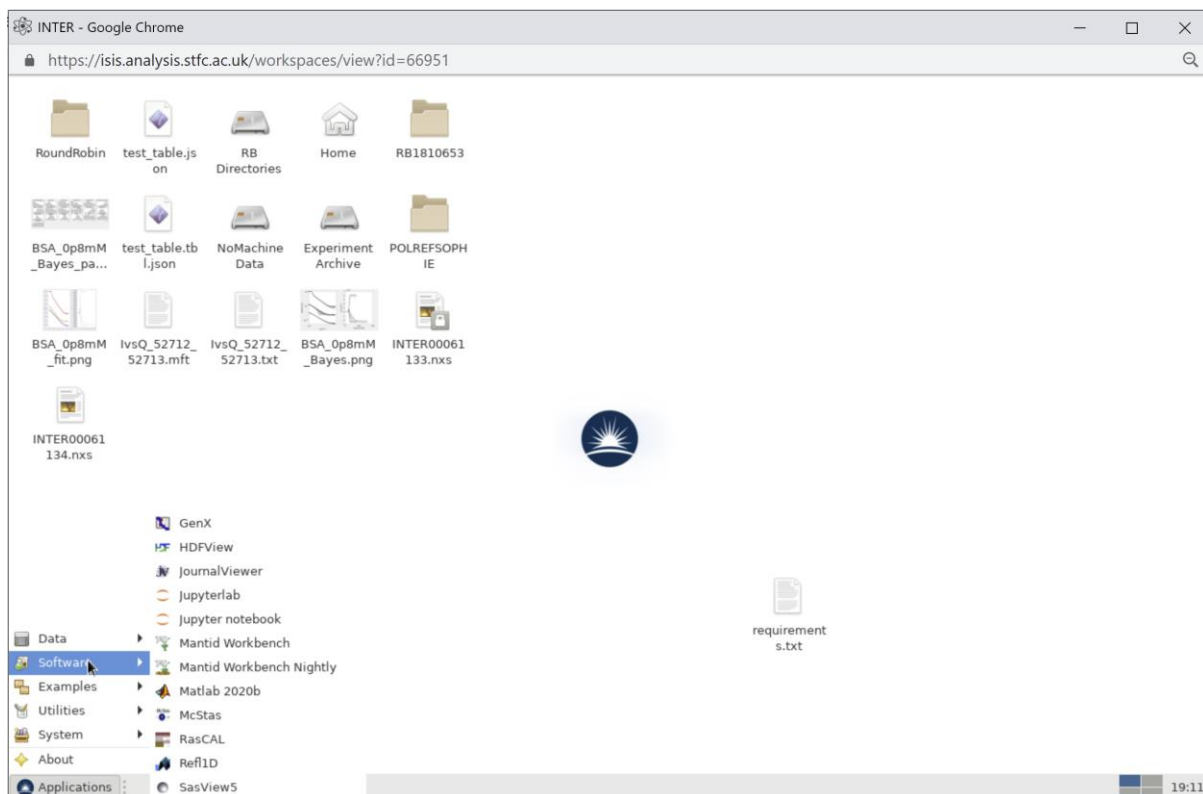
Then, create a new environment by selecting



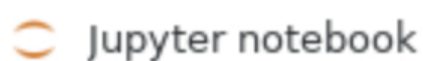
From the list of instruments select “INTER”, then “CREATE WORKSPACE” and finally hover and open in new window:



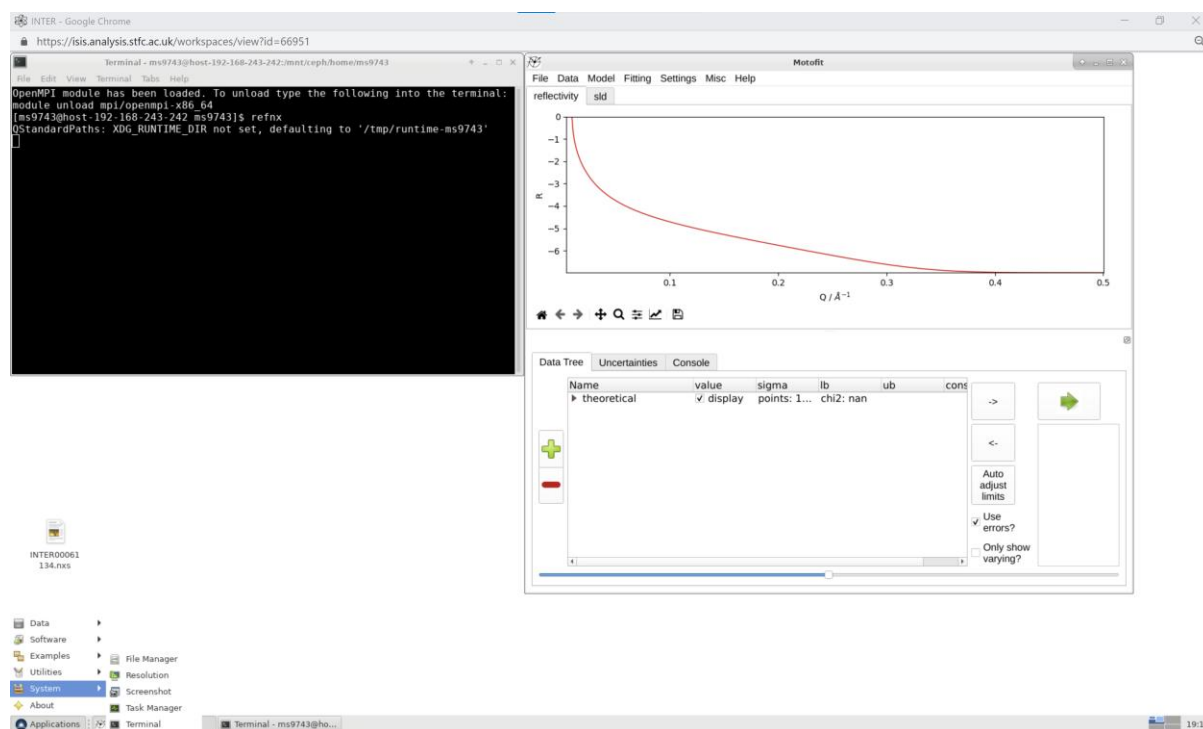
A new window with a Desktop environment will open. From the “Applications” menu in the bottom left corner, you will be able to launch various software packages:



Please check well ahead of the course, whether you can launch the following applications:



In addition, launch a Terminal from “Applications->System->Terminal” and enter “**refnx**” (no quotes) into the console. You should get a window titled “Motofit”:



## 5 ONLINE RESOURCES

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For some of the demonstrations, we will use freely available online resources. You may find these also useful after the course, when preparing or analyzing a reflectivity experiment. You may also like to try some of these before or during the course. Here is a list:

1. <https://pages.nist.gov/reflectometry-calculators/reflectivity-calculator.html>  
**NIST** online reflectivity calculator and fitting interface. This is a perfect web interface for getting a more intuitive feeling of how sample parameters influence the shape of the reflectivity curves. It is also useful for quickly fitting simpler data sets, as it requires no installed software. We will be using this interface for **Practical/demo 1/2**.
2. <https://www.ncnr.nist.gov/resources/activation/>  
Another really useful online resource from **NIST**. It allows the calculation of scattering length densities of any material.
3. <https://www.mantidproject.org/>  
Mantid data analysis software website.
4. <https://refl1d.readthedocs.io/en/latest/pdf/>  
Documentation for the Refl1D fitting software.
5. <https://refnx.readthedocs.io/en/latest/>  
Documentation for the RefNX fitting software. See also video tutorials therein.
6. <http://pslsc.isis.rl.ac.uk/>  
**BSLDC** - (The Biomolecular neutron scattering length density calculator) from **ISIS** - which determines the "match points" of biomolecules, specifically peptide / protein, DNA and RNA, in D<sub>2</sub>O : H<sub>2</sub>O mixtures or with increasing levels of deuteration. The calculator also provides a number of other parameters, including chemical composition, molecular weight (Mw), estimated volume (as a sum of the components) and an estimate of the forward (also called zero angle) intensity ( $I(0)$ ) of the biomolecule.

## 6 OWN PROBLEM SUBMISSION

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For those of you, who have already performed reflectivity experiments, we would like to offer you the opportunity to discuss your own data analysis. Given the potentially high number of requests, we may not be able to accommodate all requests, but we will do our best.

For the best support, we need to know as much as possible about the data you wish to discuss. Please provide the following information, no later than **12<sup>th</sup> of November**:

1. Polarised or unpolarised
2. Instrument where data were taken
3. Brief experiment description
4. Sample description (as much information as possible about assumed layer structure)
5. Fitting software used (if any)
6. Any other useful information