

ISIS Virtual Reflectivity Training Course

Report of Contributions

Contribution ID: 1

Type: **not specified**

Lecture 1: Introduction to reflectometry

Tuesday, 16 November 2021 09:15 (45 minutes)

- Scattering theory
- Optical matrix
- Examples

Presenter: WEBSTER, John (STFC)

Session Classification: Morning Session

Contribution ID: 2

Type: **not specified**

Lecture 2: Unpolarised Reflectometry - all you need to know

Tuesday, 16 November 2021 10:15 (1 hour)

- Experimental design
- SLD calculation
- Dynamic range and resolution
- Isotopic Contrast
- Examples

Presenter: CLIFTON, Luke (STFC)

Session Classification: Morning Session

Contribution ID: 3

Type: **not specified**

Practical 1/2: Demonstration and first model

Tuesday, 16 November 2021 11:30 (45 minutes)

NIST Online tool demo and fitting of RR sample

Presenter: SKODA, Maximilian (STFC)

Session Classification: Morning Session

Contribution ID: 4

Type: **not specified**

Lecture 3: Polarised Reflectometry - all you need to know

Tuesday, 16 November 2021 13:50 (55 minutes)

Presenter: KINANE, Christy (STFC)

Session Classification: Afternoon Session

Contribution ID: 5

Type: **not specified**

Practical 3: PNR demonstration and first model

Tuesday, 16 November 2021 15:00 (45 minutes)

NIST online demo and fitting - PNR/PA

Presenter: CARUANA, Andrew (STFC)

Session Classification: Afternoon Session

Contribution ID: 6

Type: **not specified**

Lecture 4: Data reduction

Thursday, 18 November 2021 09:00 (50 minutes)

- Basic beamline set-up
- Virtual beamline tour
- Time-Of-Flight
- Data reduction in Mantid WorkBench

Presenter: SKODA, Maximilian (STFC)

Session Classification: Morning Session

Contribution ID: 7

Type: **not specified**

Practical 4: Data reduction with Mantid in IDAaaS

Thursday, 18 November 2021 10:00 (1 hour)

- IDAaaS introduction
- Data access
- Data reduction steps
- Reflectometry interface

Presenters: SKODA, Maximilian (STFC); HALL, Stephen (STFC)

Session Classification: Morning Session

Contribution ID: 8

Type: **not specified**

Lecture 5: Data reduction II - Jupyter Notebook

Presenter: CARUANA, Andrew (STFC)

Session Classification: Morning Session

Contribution ID: 9

Type: **not specified**

Practical 5: Jupyter Notebook

Presenter: CARUANA, Andrew (STFC)

Session Classification: Morning Session

Contribution ID: **10**

Type: **not specified**

Lecture 5: Fitting - general introduction

Thursday, 18 November 2021 11:15 (45 minutes)

- Fitting basics (Fourier transform, phase loss etc.)
- Model parametrisation:
- Slab models
- Custom models
- Fitting pitfalls

Presenter: MCCLUSKEY, Andrew (ESS)

Session Classification: Morning Session

Contribution ID: 11

Type: **not specified**

Practical 5/6a: RasCAL in IDAaaS Demo

Thursday, 18 November 2021 14:30 (1 hour)

RascAL fitting/error analysis demo and simple practical

Presenter: HALL, Stephen (STFC)

Session Classification: Afternoon Session

Contribution ID: 12

Type: **not specified**

Lecture 6: Error analysis

Thursday, 18 November 2021 13:30 (45 minutes)

- Why error analysis?
- Bayesian analysis
- Model selection

Presenters: CARUANA, Andrew (STFC); MCCLUSKEY, Andrew (ESS)

Session Classification: Afternoon Session

Contribution ID: 13

Type: **not specified**

Practical 7a: RasCAL/IDAaaS error analysis demo

RasCAL error analysis demo

Presenter: HALL, Stephen (STFC)

Session Classification: Afternoon Session

Contribution ID: 14

Type: **not specified**

Lecture 7: Case study - Lipid Bilayers

Tuesday, 23 November 2021 09:00 (30 minutes)

- RasCAL revisited
- Building a model
- Custom models
- Fitting strategies and pitfalls
- Error analysis

Presenters: CLIFTON, Luke (STFC); SKODA, Maximilian (STFC)

Session Classification: Morning Session

Contribution ID: 15

Type: **not specified**

Practical 7: RasCAL Bilayer fitting

Tuesday, 23 November 2021 09:30 (2h 30m)

Building bilayer models

Presenters: CLIFTON, Luke (STFC); HALL, Stephen (STFC); SKODA, Maximilian (STFC); WELBOURN, Becky (STFC); CAMPANA, Mario (STFC)

Session Classification: Morning Session

Contribution ID: 16

Type: **not specified**

Lecture 8: Case study - Polarised Reflectometry

Tuesday, 23 November 2021 13:15 (30 minutes)

- Measurement strategies
- Model definition
- Measurables (polarisation, spin-flip scattering, spin asymmetry)
- Error analysis

Presenters: CARUANA, Andrew (STFC); MARANVILLE, Brian; KINANE, Christy (STFC)

Session Classification: Afternoon Session

Contribution ID: 17

Type: **not specified**

Practical 8: Refl1D demo and exercises

Tuesday, 23 November 2021 13:45 (2h 30m)

- PNR
- PA
- Model Constraints

Presenters: CARUANA, Andrew (STFC); MARANVILLE, Brian; KINANE, Christy (STFC)

Session Classification: Afternoon Session

Contribution ID: **18**

Type: **not specified**

Lecture 9: Case study - Complex systems

Thursday, 25 November 2021 09:00 (30 minutes)

- Introduction to RefNX
- Building a model in RefNX
- Custom models: mixed area, non-slab models ??
- Modelling roughness
- Fitting strategies and pitfalls
- Error analysis

Presenters: NELSON, Andrew; WELBOURN, Becky (STFC); COOPER, Jos (STFC); SKODA, Maximilian (STFC)

Session Classification: Morning Session

Contribution ID: **19**

Type: **not specified**

Practical 9: RefNX demo and excersises

Thursday, 25 November 2021 09:30 (2h 30m)

- Complex models exercises

Presenters: NELSON, Andrew; COOPER, Jos (STFC); SKODA, Maximilian (STFC)

Session Classification: Morning Session

Contribution ID: 20

Type: **not specified**

Practical 10: Participant problems

Thursday, 25 November 2021 13:00 (3 hours)

Participant own problems or practice examples

Presenters: CARUANA, Andrew (STFC); HUGHES, Arwel (STFC); WELBOURN, Becky (STFC); COOPER, Jos (STFC); CLIFTON, Luke (STFC); SKODA, Maximilian (STFC); HALL, Stephen (STFC)

Session Classification: Afternoon Session

Contribution ID: 21

Type: **not specified**

Closing remarks

Thursday, 25 November 2021 16:00 (15 minutes)

- Closing remarks
- Group photo?

Presenter: SKODA, Maximilian (STFC)

Session Classification: Afternoon Session

Contribution ID: 22

Type: **not specified**

Practical 5/6b: Refl1D In IDAaaS Demo

Thursday, 18 November 2021 14:30 (1 hour)

Presenters: CARUANA, Andrew (STFC); KINANE, Christy (STFC)

Session Classification: Afternoon Session

Contribution ID: 23

Type: **not specified**

Practical 7b: Refl1D/IDAaaS error analysis Demo

Presenters: CARUANA, Andrew (STFC); KINANE, Christy (STFC)

Session Classification: Afternoon Session

Contribution ID: 24

Type: **not specified**

Welcome and introduction

Tuesday, 16 November 2021 09:00 (15 minutes)

Presenters: CLIFTON, Luke (STFC); Dr SKODA, Maximilian (STFC)

Session Classification: Morning Session

Contribution ID: 25

Type: **not specified**

The ISIS Deuteration Facility

Tuesday, 16 November 2021 13:30 (15 minutes)

Session Classification: Afternoon Session

Contribution ID: 26

Type: **not specified**

Sample Alignment Demo

Thursday, 18 November 2021 13:15 (15 minutes)

Presenter: Dr SKODA, Maximilian (STFC)

Session Classification: Afternoon Session