ISIS SANS Training Course

Tuesday, 1 February 2022 - Thursday, 10 February 2022

Programme

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Tuesday 01 February 2022

Webinars: Introduction (13:30-14:30)

time	title
13:30	Introduction to neutron scattering *Presenter: ROGERS, Sarah* - Introduction to the course - Introduction to ISIS SANS Group current staff - Introduction to Neutron Scattering ~ Basics of neutron interactions ~ Types of experiments carried out ~ Why do we do neutron scattering ~ How neutrons are made: spallation and reactor ~ Time-of-flight and wavelength distribution - Introduction to experimental hall and the SANS beamlines - The future of neutron scattering

Break (14:30-15:00)

Flash Presentations: Participant Presentations (15:00-15:50)

1-2 minute single slide presentations about research.

Break (15:50-16:10)

Flash Presentations: Participant Presentations (16:10-17:00)

1-2 minute single slide presentations about research.

Wednesday 02 February 2022

Webinars: Small-angle neutron scattering (SANS) (13:30-15:00)

time	title
13:30	Small-angle neutron scattering (SANS) part 1 *Presenter: SMITH, Gregory* - SAS from different kinds of radiation (light, electrons, X-rays, neutrons) - Momentum transfer vector, Q. How to vary Q. Relationship between Q, scattering angle, and real-space distance - Monochromatic vs time-of-flight SANS. - Scattering length density (SLD). - SANS instruments. - Instrument resolution. - SANS variants ~ Total scattering ~ VSANS. USANS. ~ SESANS.
14:00	Small-angle neutron scattering (SANS) part 2 *Presenter: SMITH, Gregory* - Reducing data ~ Going from 2D detector image to normalised 1D data. ~ Absolute cross section per unit volume. ~ General data correction sequence. ~ ISIS data reduction sequence in Mantid. ~ Measurements at ISIS to achieve normalised data. - Understanding data ~ Calculating absolute cross section per unit volume. ~ Form factors and structure factors. ~ Scattering invariant.
14:30	Small-angle neutron scattering (SANS) part 3 *Presenter: SMITH, Gregory* - Advantages of using neutrons to study materials. - Science that can be done with SANS. - Materials that can be studied with SANS. - Case studies from ISIS SANS Group.

Break (15:00-15:30)

Demos: Mantid (15:30-17:00)

time	title
15:30	Mantid *Presenter: CAVALCANTI, Leide* - Organising a Batch File after the measurements - Open Mantid in IDAaaS and Reduce Data - Show file types - Manage plots - Add runs - Slice wavelength ranges - Use Algorithms - Run a Python Script

Thursday 03 February 2022

Webinars: Data Analysis (14:00-14:50)

time	title
14:00	SANS/SAXS Data analysis *Presenter: KING, Stephen* - Purpose of data analysis - Data formats (including content, types, why they matter) - Options for data analysis - Model-fitting 101 (incl objectives, priors, optimisers, measures of fit quality) - SasView collaboration - Where to get SasView
14:45	Q&A *Presenter: KING, Stephen*

Break (14:50-15:00)

Demos: SasView (15:00-16:30)

time	title
15:00	SasView *Presenter: KING, Stephen* - Tour of the GUI - Ways to load data (files/projects/analyses, using change name) - Plotting & plot options - Linear plots - Fitting ~ P(Q) (including resolution smearing) ~ 2 column data, 3 column data, 4 column data ~ P(Q)*S(Q) (including radius effective & structure factor modes) ~ Simultaneous fitting (incl changing optimiser & using a GPU) ~ Batch fitting ~ Non-neutron data fitting - Creating models ~ Using Add/Multiply to combine 2 existing models ~ Combining more than 2 existing models ~ Creating a simple function model ~ Using an existing model as a template ~ Writing a model from scratch - Correlation function analysis - Other tools

Break (16:30-16:35)

Webinars: Data Analysis (16:35-17:00)

time	title
16:35	Q&A *Presenter: KING, Stephen*

Friday 04 February 2022

Advanced measurement and data analysis methods: Webinars and Demos (13:30-17:00)

time	title
13:30	Introduction to SESANS *Presenter: DALGLIESH, Robert*
14:00	Multiple scattering in MuScatt/SASfit *Presenter: SMITH, Gregory*
14:30	SASSIE: atomistic modelling *Presenters: DOUTCH, James, MAHMOUDI, Najet*
15:00	Break
15:30	Free-Form Modelling *Presenter: KING, Stephen*
16:00	McSAS software *Presenter: KING, Stephen*
16:30	ffsas software *Presenter: KING, Stephen*

Monday 07 February 2022

Webinars: Real-space analysis of SANS data (13:30-15:00)

time	title
13:30	SANS of biological systems *Presenters: DOUTCH, James, MAHMOUDI, Najet* - Contrast variation: isotopic and perdeuteration - Sample preparation - Examples of biological complexes ~ Dilute protein solutions; globular and IDP in lipid mimics ~ Protein complexes ~ Protein/nucleotides complexes ~ Lipid nanoparticles - Analysis of biological SANS ~ Theory of real-space analysis ~ Shape reconstruction ~ Atomistic and coarse-grained modelling ~ Integrative approaches to solution structure analysis

Break (15:00-15:30)

Demos: Real-space software (15:30-17:00)

time	title
15:30	Real-space software *Presenters: DOUTCH, James, MAHMOUDI, Najet* - Scatter: Guinier plots, Porod volume, Kratky plots, Invariant analysis - ATSAS: calculation of P(r), DAMMIN and DAMMIF - MulCH: basis spectra decomposition from contrast-variation series - p(r) in SasView.

Tuesday 08 February 2022

Webinars: Scattering from magnetic and ordered systems (13:30-15:00)

time	title
13:30	Scattering from ordered and magnetic systems part 1 *Presenter: HONECKER, Dirk* - Orientational distributions of particles ~ Measure the degree of orientational order ~ 2D inversion method to analyse anisotropic small-angle scattering ~ Revisit structure factor of particle assemblies (Self-assembly, partially ordered arrays of particles, mesocrystals) - Small-angle diffraction (skyrmions, flux-line lattices) ~ Ewald sphere and area detector ~ Rocking Scans ~ Correlation function analysis (What is in the peak width, instrumental resolution)
14:15	Scattering from ordered and magnetic systems part 2 *Presenter: ALBA VENERO, Diego* - The different kinds of scattering (coherent, incoherent, elastic, inelastic, nuclear spin incoherent) - Introduction to Neutron Spin, Polarisation and Magnetic Scattering - Halpern Johnson vector - Examples

Break (15:00-15:30)

Demos: Magnetic/ordered software (15:30-17:00)

time	title
15:30	Mantid *Presenter: ALBA VENERO, Diego* Mantid: reducing data, selecting ROI, normalise runs, compare intensities of different diffraction spots, angular cuts.
16:15	SasView *Presenter: HONECKER, Dirk* - 2D plotting & options (e.g. sector averaging...) - 2D fitting (structural data extracting orientational distribution, batch fitting of magnetic field dependent data field) - Introduction General Scattering Calculator

Wednesday 09 February 2022

Webinars: Experimental practicalities (13:30-15:00)

time	title
13:30	Experimental practicalities part 1 *Presenter: SMITH, Gregory* - Preparing for measurements ~ Importance of preliminary information and being prepared. ~ Complementary techniques. Simultaneous SAXS and SANS. ~ Time scales. Kinetic SANS, histogram and event modes. - Contrast variation ~ Neutron SLDs. Isotopic variation. Isotope effects. ~ Deuteration chemistry. Other isotopic labeling. ~ Simultaneous data fitting.
14:15	Experimental practicalities part 2 *Presenter: SMITH, Gregory* - Things to check during measurements ~ Wavelength slicing in ToF SANS. ~ Incoherent and inelastic scattering. ~ Balancing scattering and attenuation. - Sample environments ~ What kind of samples can be studied. ~ Simple sample holders for SANS (cuvettes or no cuvettes, cans). Compare to SAXS (capillaries). ~ Simple perturbations. ~ Advanced sample environments.

Break (15:00-15:30)

Demos: How to get beamtime? (15:30-17:00)

time	title
15:30	How to get beamtime? *Presenter: DALGLIESH, Robert* - How ISIS FAPs work and how to target a proposal for them as an audience. - Modes of access. - Discussing experiments with local contacts. - What to include in a proposal. What makes a good proposal.

Thursday 10 February 2022

Q&A: Feedback and Q&A with SANS Group (13:30-15:00)

Feedback and Q&A with SANS team.