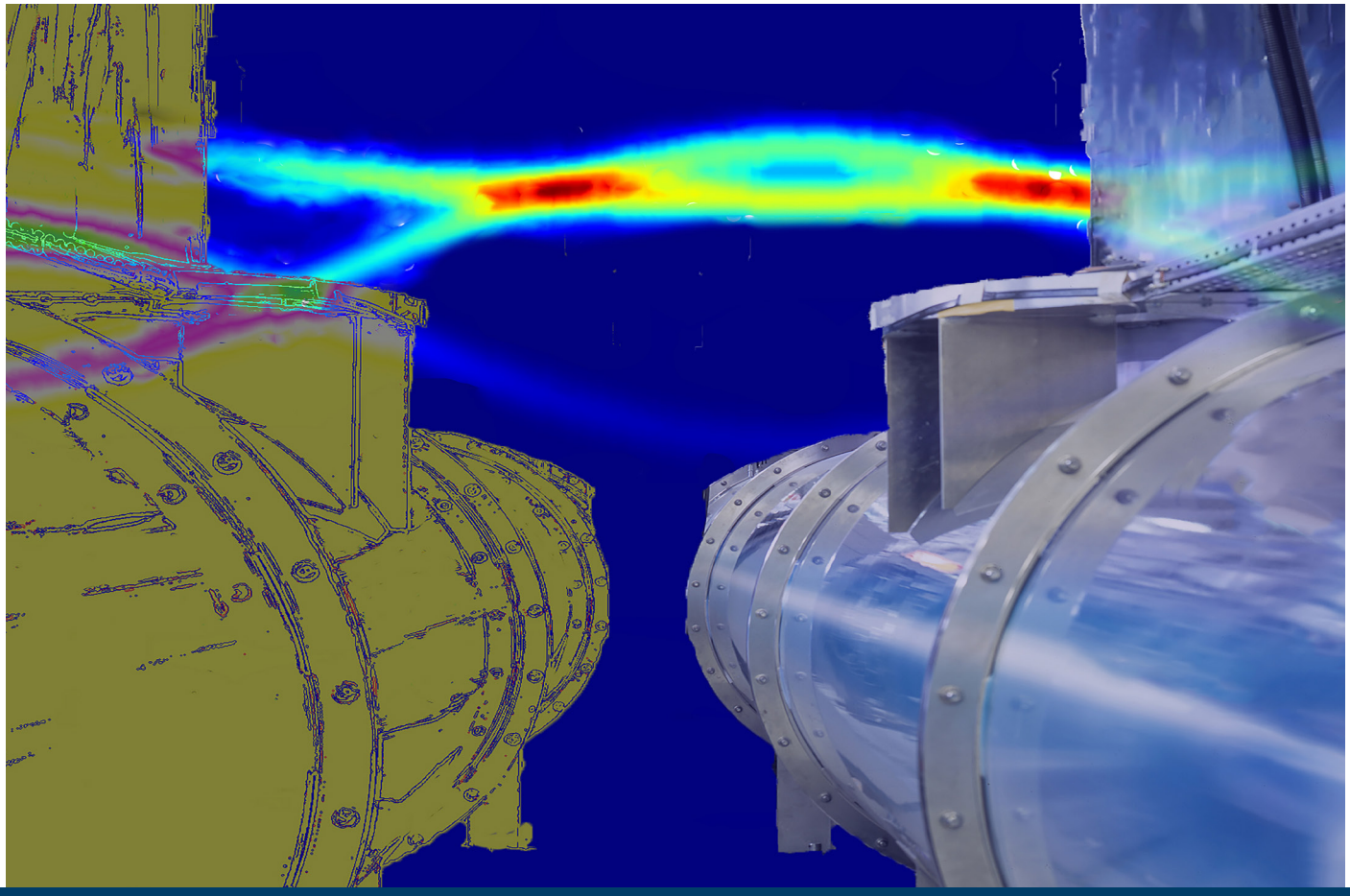


JCNS WORKSHOP 2022

TRENDS AND PERSPECTIVES IN NEUTRON SCATTERING: EXPERIMENTS AND DATA ANALYSIS IN THE DIGITAL AGE

October 11th - October 14th, 2022 | Tutzing, Germany

ABSTRACT BOOKLET

Member of the Helmholtz Association

MLZ Heinz Maier-Leibnitz Zentrum

JCNS Jülich Centre for Neutron Science

JÜLICH Forschungszentrum

Welcome to the JCNS Workshop 2022

Dear colleagues,

The digitalization has influenced the fields of neutron as well as of other scattering techniques in recent years. The application of artificial intelligence and the increasing automation of the experiments has contributed to a better use of the beam time and data, it has speeded up the data reduction, facilitated and improved the data analysis. Digital twins have also attracted much attention in neutron scattering, providing insights that can be used to better prepare experiments and train users and students. Moreover, the move from steady source to time-of-flight instrumentation as well as the passage from one- to two-dimensional detectors has triggered need for advanced and multi-dimensional data treatment. An additional challenge is to make data and software "FAIR" and sustainable.

The workshop is intended to provide a forum for software experts and neutron users to discuss these issues and to debate the challenges and opportunities of digital transformation in neutron research and related scattering techniques.

The scientific program aims to promote cross-disciplinary discussions starting from the following topics:

- Sustainable software development
- Analysis on the fly
- Inverse problems
- Experiments in the digital age
- Autonomous experiments and robotics
- AI assisted methods
- Data management
- Data reduction and analysis

The workshop is organized by the Jülich Centre for Neutron Science (JCNS) of the Forschungszentrum Jülich. The organizers like to thank all participants and hope you all will enjoy an interesting workshop.

JCNS Workshop 2022

Program overview

	Tu. Oct. 11th 2022	We. Oct. 12th 2022	Th. Oct. 13th 2022	Fr. Oct. 14th 2022
	Registration	**Session III**	**Session VI**	**Session VIII**
09:00		Brian R. PAUW	Mois I. AROYO	Andrea THORN
09:30		Gerrit GÜNTHER	Joachim WUTTKE	Zamaan RAZA
09:50		Astrid SCHNEIDEWIND	Klaus LIEUTENANT	Andrew SAZONOV
10:10		Florian RHIEM	Egor VEZHLEV	Olaf HOLDERER
10:30		Coffee break	Coffee break	Coffee break
		Session IV	**Session VII**	**Session VIII**
11:00		Eva M. HERZIG	Kuangdai LENG	Michael BUSSMANN
11:30		Tyler MARTIN	Aurel RADULESCU	Garrett GRANROTH
11:50		Michael HOFMANN	Zhanwen MA	Jakob LASS
12:10		Martin MEVEN	Christian FELDER	Rebecca FAIR
12:30	Lunch	Lunch	Lunch	Lunch
	Session I	**Session V**	**Session VII**	End of Workshop
13:40	Paolo MUTTI	Jos COOPER	Klemen VODOPIVEC	
14:10	Mario T. PARENTE	Alexander HEXEMER	Sven RANK	
14:40	Duc LE	Alexandros KOUTSIOUMPAS	Excursion	
15:00	Norberto SCHMIDT	Michael LINKE		
15:20	Coffee break	Coffee break		
	Session II	**Session V**		
16:00	Jeffrey DONATELLI	Stephan FÖRSTER		
16:30	Artur GLAVIC	Marina GANEVA		
16:50	Poster Session	Thomas WHITE		
17:10		Poster Session		
18:30-20:00	Dinner	Dinner	Workshop Dinner	

Program Timetable

Tuesday October 11th 2022

13:40 Improve neutron measurements performances with AI and machine learning
Paolo MUTTI

14:10 AI-assisted neutron spectroscopy - Log-Gaussian processes for TAS
Mario TEIXEIRA PARENTE

14:40 Machine learning for time-of-flight single crystal inelastic neutron scattering data analysis
Duc LE

15:00 Neutron instruments simulations using machine learning techniques with KDSource
Norberto SCHMIDT

15:20 Coffee break

16:00 Multi-tiered iterative projections for solving complex inverse problems from experimental data
Jeffrey DONATELLI

16:30 Reverse Monte-Carlo modeling of artificial spin systems
Artur GLAVIC

16:50 Poster Session

18:30 Dinner

Wednesday October 12th 2022

09:00 A holistic workflow for extracting excellent structural information at high rates from a short-staffed X-ray scattering laboratory
Brian Richard PAUW

09:30 Toward a digital twin at the NeXus file level
Gerrit GÜNTHER

09:50 DAPHNE4NFDI – towards FAIR and sustainable neutron and photon data
Astrid SCHNEIDEWIND

10:10 SampleDB: a web-based electronic lab notebook with a focus on sample and measurement metadata
Florian RHIEM

10:30 Coffee break

11:00 Towards real-time analysis and structural control using in-situ characterization of thin film processing
Eva M. HERZIG

11:30 The nSoft autonomous formulation laboratory: X-ray and neutron scattering for industrial formulation discovery
Tyler MARTIN

11:50 High accuracy neutron diffraction measurement using an industrial robot system at the STRESS-SPEC instrument
Michael HOFMANN

12:10 Adaptive data acquisition at the hot single crystal diffractometer HEiDi at MLZ: What do we have and what will we need in the future?
Martin MEVEN

12:30 Lunch break

13:40 Maximising information gain and optimizing experimental design for neutron reflectivity
Jos COOPER

14:10 Bringing Machine Learning to Beamline
Alexander HEXEMER

14:40 Automated software and advanced tools for treating small-angle scattering and reflectivity data from bio-molecular structures
Alexandros KOUTSIOUMPAS

15:00 Storage and Infrastructure for Big Data and AI
Michael LINKE

15:20 Coffee break

16:00 Fast Calculation of Scattering Patterns Using Hypergeometric Function Algorithms
Stephan FÖRSTER

16:30 Classification of Small-Angle Scattering Patterns Using Machine Learning on Transformed 2D-Data
Marina GANEVA

16:50 Real-time data processing for serial X-ray crystallography
Thomas WHITE

17:10 Poster Session

18:30 Dinner

Thursday October 13th 2022

09:00 Online material studies by the Bilbao Crystallographic Server
Mois I. AROYO

09:30 Ten years Scientific Computing Group at MLZ - our quest for sustainable data analysis software
Joachim WUTTKE

09:50 The new versions 3.5 and 4.0 of the instrument simulation program VITESS
Klaus LIEUTENANT

10:10 Particle transport codes simulations for the design of the HBS Target-Moderator-Reflector assembly
Egor VEZHLEV

10:30 Coffee break

11:00 Quantifying structural ambiguity from polydisperse parameter inversion in small-angle scattering
Kuangdai LENG

11:30 Materials informatics approach on neutron scattering data for the development of anion exchange membranes used for next-generation
Aurel RADULESCU

11:50 VITESS simulation and virtual experiment of the neutron diffractometer for small samples at the High Brilliance Neutron Source
Zhanwen MA

12:10 Leveraging containerization technology for FAIR data management
Christian FELDER

12:30 Lunch break

13:40 Modernizing SNS Neutron Scattering Instruments with proven Control System tools
Klemen VODOPIVEC

14:10 Open Science at Forschungszentrum Jülich (OS4FZJ)
Sven RANK

15:00 Excursion and Workshop dinner

Friday October 14th 2022

09:00 Diagnostics for Macromolecular Structure Determination at Neutron Sources: AUSPEX
Andrea THORN

09:30 Single crystal neutron diffraction data reduction with OpenHKL
Zamaan RAZA

09:50 Simplifying diffraction data analysis with EasyDiffraction
Andrew SAZONOV

10:10 Efficient data extraction with automated report generation for neutron spin echo raw data
Olaf HOLDERER

10:30 Coffee break

11:00 Fusing HPC and Edge – Making optimum use of knowledge
Michael BUSSMANN

11:30 Monte Carlo ray tracing simulations for comparison to neutron scattering experiments
Garrett GRANROTH

11:50 MJOLNIR: Data treatment of CAMEA-like multiplexing instruments
Jakob LASS

12:10 Euphonic: efficient inelastic neutron scattering simulations and more from force constants
Rebecca FAIR

12:30 Lunch break

13:30 End of Workshop

Abstracts

Tuesday, October 11th 2022

Tuesday, October 11th 2022, 13:40-14:10

Improve neutron measurements performances with AI and machine learning

Paolo MUTTI[1], Martin BOEHM[1], Yannick LE GOC[1], Tobias WEBER[1], Marcus NOACK[2], James SETHIAN[2]

[1]Institut Laue-Langevin, Grenoble, France

[2] Lawrence Berkeley National Laboratory, Berkeley, United States

Artificial Intelligence and machine learning are, nowadays, powerful methods to increase the performances of neutron scattering experiments. In the present talk we will present two different use-cases covering both aspects. Small Angle Neutron Scattering (SANS) is a growing technique especially in biology and it is characterized by short measuring time and, therefore, high throughput of samples per experiment. This high-volume data contains rich scientific information about structure and dynamics of materials under investigation. We applied deep learning techniques to evaluate the quality of experimental neutron scattering images [1], which can be influenced by instrument configuration, sample and sample environment parameters. Sample structure can be deduced on-the-fly during data collection that can be therefore optimised. A three-axis neutron spectrometer represent the opposite situation in terms of quantity of collected data although an experiment last typically several days. It is therefore crucial to concentrate the data acquisition in those regions of the reciprocal space where a maximum of information can be acquired. In autonomous learning, algorithms learn from a comparatively little amount of input data and decide themselves on the next steps to take in a closed-loop. We have performed a series of experiments fully driven by the computer without any human intervention. The used algorithm was able to explore the reciprocal space and fully reconstruct the signal without any prior knowledge of the physics case under study. Thanks to autonomous learning, gpCAM, developed by Marcus Noack of the CAMERA team at Berkeley Lab, estimates the posterior mean and covariance and uses them in a function optimization to calculate the optimal next measurement point. The main advantage of such an approach is clearly the possibility to drastically reduce the number of measurements with respect to a classical grid scan (i.e. const- Q, const-E scans) and therefore optimize the beam-time usage [2]. In this talk we will compare these new experimental approaches and compare them to traditional data acquisition. We try to show a perspective of the future possibilities and how the scientific measurements could evolve in conjunction with modern algorithms.

[1] J. Schmidhuber, Neural networks, **61**, 85 (2015).

[2] M.M. Noack, M.M., Zwart, P.H., Ushizima, D.M. et al., Nat. Rev. Phys., **3**, 685 (2021).

E-mail of the corresponding author: mutti@ill.fr

Tuesday, October 11th 2022, 14:10-14:40

AI-assisted neutron spectroscopy - Log-Gaussian processes for TAS

Mario TEIXEIRA PARENTE[1], Georg BRANDL[1], Astrid SCHNEIDEWIND[1], Christian FRANZ[1], Uwe STUHR[2], and Marina GANEVA[1]

[1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich, Garching, Germany

[2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland

Three-axes spectroscopy (TAS) is a well-established method that has not substantially changed in the past decades of its use. Nowadays, with increasing demand and limited availability of TAS instruments, application of AI methods is one option to increase the efficiency of TAS. From the perspective of an AI method, TAS experiments collect noisy observations of a 2D intensity function to investigate a material of interest. If the material's intensity structure is unknown, experimenters usually decide manually where to place measurements for a rapid overview. AI methods can assist this process by choosing informative measurement locations while taking instrument costs into account and hence optimize the available beam time in this mode. For example, avoiding measurements in the background (no signal) but preferring regions of signal leads to more efficient measurements. Our method [1] for discovering regions of signal is based on Gaussian Process Regression as a technique for probabilistic function approximation and makes use of log-normal distributions. Moreover, it considers different moving times for energy- / Q-scans, handles noise and background functions, and respects weak as well as strong intensities to avoid loss of information. For example, for simple dispersions like intensity-modulated phonons, full information can be achieved only within a reasonably short amount of experimental time. The algorithm was tested on simulated data for several typical functions (CEF, phonons, SDW, dispersion of frustrated systems) and experimentally on EIGER/PSI. In order to quantify the benefit of our approach, we present results of a benchmarking procedure [2] that we have developed as a cost-benefit analysis in a synthetic but still representative setting.

[1] Teixeira Parente M., Brandl G., Schneidewind A., Noack M., Boehm M., Ganeva M., arXiv e-prints, 2105.07716 (2021).

[2] Teixeira Parente M., Schneidewind A., Brandl G., Noack M., Boehm M., Ganeva M., Front. Mater. 8, 772014 (2022).

E-mail of the corresponding author: m.teixeira.parente@fz-juelich.de

Tuesday, October 11th 2022, 14:40-15:00

Machine learning for time-of-flight single crystal inelastic neutron scattering data analysis

Duc LE[1], Deniza Chekrygina[2], Keith Butler[2], Samuel Jackson[2], Jeyan Thiyagalingam[2], Toby Perring[1]

[1]ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, OX11 0QX, UK

[2]Scientific Computing Department, STFC Rutherford Appleton Laboratory, OX11 0QX, UK

Recent trends have seen the sizes of time-of-flight single crystal inelastic neutron scattering (INS) measurement datasets grow progressively larger, as spectrometers get bigger or use multiplexing techniques to acquire more data simultaneously. As such, the data analysis has grown more complex, taking longer to complete.

Machine learning (ML) may be applied to make this process easier. But, while individual datasets may be large, there are relatively few measured datasets available for training because of the long counting times required per experiment. Thus, standard ML techniques which tend rely on large numbers of datasets of modest sizes ("big data") cannot be used directly. One way around this is to use synthetic data from atomistic calculations of the sample's behaviour, for example to train a convolution neural network (CNN) to classify spin-wave models [1]. We have recently extended this work to train the network to act as a surrogate model – that is, to reproduce the atomistic simulations in a fraction of the time of the original calculations. These approximate spectra can then be used with traditional fitting techniques, and the fitted parameters verified with the full atomistic calculations.

Using atomistic calculations to generate spectra for training limits the applicability of the trained network to a particular material or class of materials, however. In addition, the spectra may contain signals from the sample holder or environment, or other artefacts which are not accurately modeled. These use cases have traditionally been handled by manually inspecting the data, a process which can take months or longer. In this work, we also explore the use of unsupervised learning techniques such as clustering and gaussian mixture models for segmenting large datasets between different kinds of signals (from sample magnetic or lattice scattering, or from the sample environment) and background, which could be used to quickly narrow down regions of interest in large datasets.

[1] K. T. Butler et al., J. Phys.: Condens. Mater., **33**, 194006 (2021)

E-mail of the corresponding author: duc.le@stfc.ac.uk

Tuesday, October 11th 2022, 15:00-15:20

Neutron instruments simulations using machine learning techniques with KDSource

N.S. SCHMIDT[1,2], O.I. Abbate[3], Z.M. Prieto[3], J.I. Robledo[3], J.I. Márquez Damián[4], A.A. Márquez[2,3], J. Dawidowski[2,3], E. Mauerhofer[1], T. Gutberlet[1], T. Brückel[1]

[1] Jülich Centre For Neutron Science, Forschungszentrum Jülich, Jülich, Germany
[2] Instituto Balseiro, Universidad Nacional de Cuyo, S. C. de Bariloche, Argentina
[3] Comisión Nacional de Energía Atómica, S. C. de Bariloche, Argentina
[4] European Spallation Source ERIC, Lund, Sweden

The design of neutron instruments usually is related to the simulations of neutron beams. These simulations are normally decoupled from the neutron source since the nuclear reactions that govern the generation of neutrons in the source are independent of the specific interactions that take place in the neutron beam path. Also, neutron beams are usually transported far away from the source to reduce the background signal in the measurements and the radiation dose of the personnel. When evaluating the neutron beam under different operating conditions, it is useful to have a source that can be re-sampled.

KDSource [1,2] is an open-source code that uses the adaptive multivariate Kernel Density Estimation (KDE) method to estimate the source distribution at a given point in the beam trajectory, which seeks to overcome limitations of other variance-reduction techniques. The approach presents a novel methodology to optimize source modelling, which may be especially suited for neutron beam and radiation shielding simulations.

The core idea of the methodology is to use some machine learning libraries and algorithms to optimize the bandwidth selection for each source variable. With this strategy, smooth estimates of the variable distributions may be obtained from particle lists at a given point in a simulation that maintains correlations among all the variables. The code implements the proposed methodology in Python, and it consists of a module for KDE model optimization, and another for sampling (i.e. generating new particles using the previously optimized model).

This work aims to present the KDSource code with some usage examples to design the neutron imaging instruments for the HBS project.

[1] N.S. Schmidt, O.I. Abbate, Z.M. Prieto, J.I. Robledo, J.I. Márquez Damián, A.A. Márquez, J. Dawidowski, 2022. KDSource, a tool for the generation of Monte Carlo particle sources using kernel density estimation. Ann. Nucl. Energy 177.
URL: https://doi.org/10.1016/j.anucene.2022.109309
[2] O.I. Abbate, N.S. Schmidt, Z.M. Prieto, J.I. Robledo, J.I. Márquez Damián, A.A. Márquez, J. Dawidowski, 2021. KDSource, a tool for the generation of Monte Carlo particle sources using kernel density estimation. GitHub repository.
URL: https://github.com/KDSource/KDSource

E-mail of the corresponding author: no.schmidt@fz-juelich.de

Tuesday, October 11th 2022, 16:00-16:30

Multi-tiered iterative projections for solving complex inverse problems from experimental data

Jeffrey DONATELLI[1,2]

[1]Mathematics Department, Lawrence Berkeley National Laboratory, Berkeley, USA

[2]Center for Advanced Mathematics for Energy Research Applications, Lawrence Berkeley National Laboratory, Berkeley, USA

Recent upgrades at experimental facilities throughout the world are enabling several new experiments to capture properties and behavior of important biological objects and materials that were not previously possible to study. However, a major bottleneck in enabling new scientific breakthroughs from these experiments is the capability to accurately, efficiently, and robustly invert the data to reconstruct information about the sample from increasingly complex, fast, large, and sensitive detector measurements. There is a critical need to develop new math and algorithms that can accurately solve these inverse problems from new and challenging data.

I will present a new general mathematical and algorithmic framework capable of overcoming many of these challenges in inversion. This framework, called Multi-Tiered Iterative Projections (M-TIP) [1,2], is based on exploiting the multi-tiered structure inherent in many inverse problems, by breaking them up into several tiers of underdetermined subproblems, each of which can be solved efficiently via mathematical projection operations that are applied iteratively. This property allows M-TIP to leverage optimal mathematical solutions for the subproblems to improve speed, robustness, convergence, and accuracy of the overall inversion. I will demonstrate the application of this M-TIP framework in solving several important open problems in inversion from challenging data for experiments including fluctuation X-ray scattering [3,4], coherent surface scattering imaging [7], and more [5,6].

[1] J. Donatelli, P. Zwart, and J. Sethian, PNAS, **112**, 10286-10291 (2015)

[2] J. Donatelli, J. Sethian, and P. Zwart, PNAS, **114**, 7222-7227 (2017)

[3] R. Kurta, J. Donatelli et al., PRL, **119**, 158102 (2017)

[4] K. Pande, J. Donatelli et al., PNAS, **115**, 11772-11777 (2018)

[5] J. Donatelli and J. Spence, PRL, **125**, 065502 (2020)

[6] Z. Hu, J. Donatelli, and J. Sethian, PNAS, **118**, e2105826118 (2021)

[7] J. Donatelli, M. Chu, N. Schwarz, Z. Jiang, and J. Sethian (In preparation)

E-mail of the corresponding author: jjdonatelli@lbl.gov

Tuesday, October 11th 2022, 16:30-16:50

Reverse Monte-Carlo modeling of artificial spin systems

Artur GLAVIC[1], Gavin M. MACAULEY[2], Jonathan WHITE[3]

[1]Laboratory for Neutron and Muon Instrumentation,

[2]ETH-Zürich and Laboratory for Multiscale Materials Experiments,

[3]Laboratory for Neutron Scattering and Imaging,
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Artificially created structures of magnetic elements are model systems to investigate the long-range dipole interaction of macroscopic magnetic moments (artificial spins). The advances in nano-patterning allow us to create large 2D lattices of such magnetic elements to study geometric frustration and the resulting complex magnetic state.

On the scale between 10 and 100 nm it is hard to measure the orientation of the spins using microscopy methods but with Grazing Incidence Small Angle Scattering (GISANS) we could recently observe the magnetic structure factor in a triangular lattice of out-of-plane moments [1]. Due to the frustrated nature of the interaction, there often is no long-range magnetic order present in these systems. In our previous work, we have therefore reverted to model the inter-particle correlations using an empirical model based on theoretical predictions and implemented it in a Distorted Wave Born Approximation (DWBA) model using BornAgain [2].

A follow-up experiment showed that the magnetic correlatoins were static and not thermally active as was assumed in the theoretical models. Alterations from the theoretically predicted magnetic structure factors could therefore be expected. To analyze these datasets a model-free approach is needed. We have used the reverse Monte-Carlo (RMC) modeling technique that has already been successfully applied in neutron diffraction from bulk magnetic materials [3] and implemented it in a DWBA model to recreate the in-plane GISANS scattering that was measured on the Yoneda line at various sample orientations. The result is a real-space spin configuration that follows the physical constraints of the sample and can be used to calculate the pure spin-spin structure factor. As this approach is independent of any predictions it can be applied to many other artificial spin systems measured with GISANS.

[1] P. Pip, A. Glavic, et al., Nanoscale Horizons, **6**, 6 (2021)

[2] G. Pospelov, et al., J. Appl. Cryst., **53**, 262-276 (2020)

[3] A. Korshunov, I. Safiulina and A. Kurbakov, Phys. Status Solidi B, **257**, 1900232 (2020)

E-mail of the corresponding author: Artur.glavic@psi.ch

Data reduction graphical user interface (GUI) for DNS instrument at MLZ

Thomas MUELLER[1], **Oleksandr KOSHCHII[1]**, Marina GANEVA[1]

[1]Juelich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Juelich GmbH, Garching, Germany

Data reduction is a transformation of a dataset collected during a neutron scattering experiment into a dataset in physical units. This process requires detailed knowledge of geometry and configuration of the instrument at which the dataset was accumulated. As a result, data reduction is among the most important and complex stages that researchers have to work on in order to link raw experimental data to a meaningful scientific publication.
In our work, we developed a GUI that will help instrument scientists and users of the DNS instrument at MLZ to optimize their data reduction workflow and perform it in a user-friendly and simplified way. The interface implements a set of data reduction algorithms and can be used for different types of experimental measurements at DNS. More specifically, the GUI contains the following modes of data reduction: time-of-flight (TOF) powder diffraction, elastic powder, single crystal elastic and simulation. The interface not only will be fully integrated into the popular Mantid [1] framework but also can be used in a standalone autonomous way.

[1] O. Arnold, et al., Nucl. Instrum. Methods Phys. Res. A, **764**, pp. 156-166 (2014).

E-mail of the corresponding author: o.koshchii@fz-juelich.de

Estimation of diffusive properties for *in*-silico materials using a Gaussian process to complement quasi-elastic neutron scattering measurements

Andrew R. MCCLUSKEY[1], Samuel W. COLES[2], Benjamin J. MORGAN[2], Daria NOFERINI[1]

[1]European Spallation Source ERIC, P.O. Box 176, SE-221 00, Lund, Sweden

[2]Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK

Quasi-elastic neutron scattering (QENS) is a popular tool for the experimental study of diffusion in solid-state materials [1]. Commonly, the results from QENS measurements are interpreted alongside complementary molecular dynamics simulations [2, 3]. However, the high computational cost of these simulations, in particular for *ab-initio* methods, limits both the system size and timescale, meaning it is only possible to estimation the diffusion coefficient. Frequently, the diffusion coefficient is estimated without reporting of uncertainty, that would be observed if the simulation were repeated. Without a well-defined uncertainty analysis, it is not possible to compare between calculated values and those derived from experimental methods such as QENS. To address this, we have developed a robust methodology, using bootstrap resampling and a first-principles approach to generate a Gaussian process that describes the mean-squared displacement of particles diffusing in a material. This is capable of obtaining a statistically efficient estimate of the diffusion coefficient and an accurate estimate of the associated uncertainty. In this work, we will present this methodology and show its application in materials science, enabling comparison with experimental QENS data. This methodology has been made available as an open-source Python package, kinisi (kee-nee-see) [4], with documentation at kinisi.rtfd.io.

[1] A. R. Shah, *et al.*, *J. Phys. Mater.*, **4**, 042008 (2021).

[2] Q. Chen, *et al.*, *J. Mater. Chem. A.*, **8**, 25290 (2020).

[3] M. K. Gupta, *et al.*, *Phys. Rev. Mater.*, **4**, 045802 (2020).

[4] A. R. McCluskey & B. J. Morgan, kinisi (Version 0.3.9) [Computer software], 2021. url: https://github.com/bjmorgan/kinisi

E-mail of the corresponding author: andrew.mccluskey@ess.eu

Exploiting symmetry with brille

Gregory S. TUCKER[1]

[1]European Spallation Source ERIC, P.O. Box 176, SE-221 00, Lund, Sweden

The properties of crystalline materials are studied by various means including inelastic neutron scattering (INS), always with the goal of increased understanding of the material in question and often aiming to apply knowledge gained more broadly. All such properties are con-strained to be periodic with the period of the crystalline lattice which typically includes translational and rotational symmetries. The periodic unit of the lattice is the irreducible Brillouin zone (irBz), and INS measurements are able to collect intensity over many such equivalent volumes of momentum-space.

Extracting the underlying physical properties of the material typically requires use of a model system, often implemented as a computer program which calculates intensities for a series of fixed positions in momentum-space. These calculations must also be periodic over the lattice and the programs typically cannot easily be scaled-up to calculate for all independent momentum-space positions probed in an INS measurement.

A computer program, brille, has been created in order to support the fitting of such models to measured INS data. It handles finding the irBz volume for a lattice, creates a space-filling grid within the identified irBz, and identifies equivalent momentum-space points within the irBz for arbitrary momentum-space points. Additionally, brille can hold user-provided data at the vertices of the space-filling grid and subsequently interpolate at arbitrary irreducible momentum-space points.

The interpolated results at a point in the irBz are not strictly identical to what a model would calculate at the equivalent momentum-space point. In such a case the results are related by the symmetry operation which relates the irreducible and non-irreducible points and, if the relationship is known and provided, brille can provide the correct results up to approximations caused by the linear interpolation for arbitrary momentum-space points. Thus far, brille supports the correct handling of the eigenvectors and eigenvalues of the grand dynamical matrix and can be used along with, e.g., Euphonic, to provide linear interpolated phonon modes and intensities from electronic structure calculations.

By interpolating model values at arbitrary momentum points, brille can lessen the work re-quired of the model functions and improve simulation and fitting times of full INS data sets.

E-mail of the corresponding author: gregory.tucker@ess.eu

Commissioning standardized formats for tomography data collection and reconstruction

Stefanos ATHANASOPOULOS[1], Søren SCHMIDT[1], Tobias RICHTER[1]

[1]European Spallation Source ERIC (ESS), Lund, Sweden

At the European Spallation Source (ESS) the message broker system Apache Kafka will be used as raw data event streaming platform [1]. All data will be streamed live and compiled into NeXus format data files [2]. Data processing can operate both on the live data stream and the NeXus files. With the ESS accelerator and target still under construction, Ymir, a lab instrument, has been set up for device testing and controls integration without neutrons. Ymir is being used to establish the infrastructure for recording and time-stamping of all relevant information for any measurement. Like any instrument at ESS, it also uses the experiment control software NICOS [3] for the orchestration of the data acquisition.

This presentation covers the optical light tomography setup at Ymir, which has been designed to demonstrate and commission the ESS data pipeline for instruments. From a data and controls point of view, the optical light setup exposes equivalent characteristics to those of a neutron or X-ray instrument, fully complying with the principles of tomography, and uses identical components, including imaging detectors (i.e., cameras).

The main focus of the present work is on the live tomography data streaming process though Kafka and the NeXus file compilation. Various challenges are discussed and future objectives in relation to ESS' multi-purpose imaging instrument, ODIN, are outlined, such as the dual mode tomography feature that will involve the combined employment of neutrons and X-rays.

[1] https://kafka.apache.org

[2] https://www.nexusformat.org

[3] https://nicos-controls.org

E-mail of the corresponding author: stefanos.athanasopoulos@ess.eu

POWTEX: Angular- and Wavelength-Dispersive High-Intensity Neutron TOF Diffractometer

Yannick MEINERZHAGEN[1], Andreas HOUBEN, Richard DRONSKOWSKI[1]

[1] Chair of Solid-State and Quantum Chemistry, Institute of Inorganic Chemistry, RWTH Aachen University, D-52056 Aachen, Germany

POWTEX is a future TOF neutron powder diffractometer [1] under construction at MLZ. Funded by Germany's Federal Ministry of Education and Research (BMBF), POWTEX is built by RWTH Aachen University and FZ Jülich, with contributions for dedicated texture sample environments from the Geoscience Center of Göttingen University. We will present an overview of the instrument and the advances made in neutron instrumentation, too. Several new concepts were developed, including a novel ^{10}B detector [2] and a double-elliptic neutron-guide system sharing focal points at the positions of pulse chopper and sample.
POWTEX aims for rapid measurements and will give access to *in situ* chemical experiments, e.g., phase transitions as a function of temperature, pressure, and magnetic field. The large angular coverage of nine steradian drastically reduces the need for sample tilting/rotation when it comes to texture analysis, *in situ* deformation, annealing, simultaneous stress, etc. As the POWTEX instrument collects angular- and wavelength-dispersive data (intensity as a function of both 2θ and λ), we are currently extending the Rietveld approach to process two-dimensional data. To create data sets for this purpose, we implemented the algorithm *PowderReduceP2D* into the data-reduction software Mantid [3]. In addition, new refinement algorithms for an in-house version of the commonly used refinement software GSASII [3, 4, 5] were developed and applied. The first results for data collected with a single detector module of POWTEX at the POWGEN instrument (SNS, ORNL) will be shown [3]. These data were reduced with the new Mantid algorithm and then two-dimensionally refined, yielding a new perspective on the Rietveld method.
Also, to better visualize data sets depending on two variables, the 2θ and λ coordinate system was analytically converted into a new rectangular d and $d_\perp$ coordinate system, thereby representing the sinusoidal reflection curves into straight lines located on a fixed d position [4].

[1] H. Conrad, Th. Brückel, W. Schäfer, J. Voigt, J. Appl. Cryst. **41**, 836 (2008).
[2] G. Modzel, M. Henske, A. Houben, M. Klein, M. Köhli, P. Lennert, M. Meven, C. J. Schmidt, U. Schmidt, W. Schweika, Nucl. Instr. Meth. A **743**, 90 (2014).
[3] A. Houben, P. Jacobs, Y. Meinerzhagen, N. Nachtigall, R. Dronskowski, https://doi.org/10.48550/arXiv.2110.12767 (2021).
[4] P. Jacobs, A. Houben, W. Schweika, A.L. Tchougréeff, R. Dronskowski, J. Appl. Cryst. **48**, 1627 (2015).
[5] P. Jacobs, A. Houben, W. Schweika, A.L. Tchougréeff, R. Dronskowski, J. Appl. Cryst. **50**, 866 (2017).

E-mail of the corresponding author: yannick.meinerzhagen@ac.rwth-aachen.de

POWTEX: Event Correlation with Pattern-Matching Algorithms

Noah NACHTIGAL[1], Andreas HOUBEN[1], Richard DRONSKOWSKI[1]

[1] Chair of Solid-State and Quantum Chemistry, Institute of Inorganic Chemistry, RWTH Aachen University, D-52056 Aachen, Germany

While anticipating the commissioning of the high-intensity time-of-flight neutron powder-diffractometer POWTEX [1, 2], significant efforts were made to optimally exploit the instrument characteristics for future multidimensional Rietveld refinements. The first test data were acquired at the POWGEN instrument of the SNS (Oak Ridge National Laboratory) using a small segment of the tailor-made POWTEX detector.

This volume-detector is actually a four-dimensional detector registering neutron events with their position (x, y, z) and time. As an improvement to conventional surface- or grid-detectors, this allows for further data-treatment possibilities. One idea, namely the event correlation, is to assign neutron events with a certain probability to one or more neutron trajectories. Such trajectories, i.e., rays of neutrons describing a very similar scattering process, can be projected back to their origin. By doing so, neutron events from the sample are separable from those neutrons originating from other scatterings sources, e.g., the sample environment. This would in turn facilitate removing background from the data. In one preliminary approach, we used pattern-matching algorithms such as Random Sample Consensus (RANSAC) [3] and Hough Transform [4] to identify collinear points in the event datasets. With these algorithms, it is already possible to detect lines in a very reduced data set (around 10^6 events) that may resemble neutron trajectories. Assigning probabilities with respect to possible trajectories, however, is still a work in progress. Furthermore, the efficiency of these algorithms needs to be improved due to the immense amount of data that will be available with the full POWTEX instrument. While a total of 1.9×10^8 events were recorded within 10 hours for a single detector segment with a solid angle of about 0.23 steradians, one may expect that the solid angle multiplies to 9 steradians with the full detector. We intend to further refine these results and combine the concept with the traditional data-reduction process.

[1] H. Conrad, T. Brückel, W. Schäfer, J. Voigt, *J. Appl. Cryst.* **41**, 836–845 (2008)

[2] A. Houben, W. Schweika, T. Brückel, R. Dronskowski, *Nucl. Instrum. Methods. Phys. Res.* **680**, 124–133 (2012)

[3] M. A. Fischler, R. C. Bolles, *Commun. ACM* **24**, 381–395 (1981)

[4] R. O. Duda, P. E. Hart, *Commun. ACM* **15**, 11–15 (1972)

E-mail of the corresponding author: noah.nachtigall@ac.rwth-aachen.de

Virtual Experiments combined with Machine Learning to improve Data Evaluation of SANS measurements

José Ignacio ROBLEDO[1], Klaus Lieutenant[1]

[1]Jülich Center for Neutron Science(JCNS), Forschungszentrum Jülich (FZJ), 52425 Jülich, Deutschland

In this work we present our research line that has begun as part of the "Global Neutron Scientist" (GneuS) call N.º 1 this year. We present our strategy to combine virtual experiments with Machine Learning (ML) techniques to improve the data evaluation procedure in Small Angle Neutron Scattering (SANS) experiments. In particular, we describe the virtual experiments we are planning to do at a SANS instrument at MLZ with the VITESS software [1] to create a training database for ML algorithms, and we discuss aproposed first step exploratory analysis to the generated data using Multivariate Statistical methodologies. This analysis will give insight to the adequate ML algorithms that we will explore.

[1] C. Zendler, K. Lieutenant, D. Nekrassov, M. Fromme, Vitess 3 – Virtual Instrumentation Tool for the European Spallation, J. Phys. Conf. Ser. 528 (2014) 012036.

E-mail of the corresponding author: jorobledo2@gmail.com

Abstracts

Wednesday, October 12th 2022

Wednesday, October 12th 2022, 09:00-09:30

A holistic workflow for extracting excellent structural information at high rates from a short-staffed X-ray scattering laboratory

Brian Richard PAUW[1], Glen Jacob SMALES[1], Ingo BRESSLER[1]

[1]Unter den Eichen 87 (Bundesanstalt für Materialforschung und -Prüfung, 6.5: Synthesis and Scattering of Nanostructured Materials, Berlin, Germany)

A useful scattering experiment should eventually result in well-founded, unambiguous wide-range structural information. To get to that end requires a close look at all possible aspects that come into play when running scattering experiments, from the sample preparation to the interpretation of the analyses. This all needs to be tied together with a coherent laboratory organization to make sure your final data is FAIR, your analyses are traceable and your results are useful. Such laboratory organization can incidentally also help address the reproducibility crisis in science, and easily multiply the scientific output of a laboratory, while greatly elevating the quality of the measurements.

We have demonstrated this for small- and wide-angle X-ray scattering in the MOUSE project (Methodology Optimization for Ultrafine Structure Exploration) [1]. With the MOUSE, we have combined: a) a comprehensive and highly automated laboratory workflow with b) a heavily modified X-ray scattering instrument. This combination allows us to collect fully traceable scattering data, within a well-documented, FAIR-compliant data flow (akin to what is found at the more automated synchrotron beamlines). With two full-time researchers, our lab collects and interprets thousands of datasets, on hundreds of samples, for dozens of projects per year, supporting many users along the entire process from sample selection and preparation to the analysis of the resulting data.

Current activities are centered on mining the data catalog built up over the four years of operation, automated tagging of datasets through machine learning, and automated analyses of the data. This talk will introduce many of these aspects, and hopefully will excite a lot of questions.

[1] Smales, G. J, and Pauw, B.R., Journal of Instrumentation, **16**, P06034 (2021).

E-mail of the corresponding author: Brian.pauw@bam.de

Wednesday, October 12th 2022, 09:30-09:50

Toward a digital twin at the NeXus file level

Gerrit GÜNTHER[1], Simone VADILONGA[1], Peter BAUMGÄRTEL[1], Oonagh MANNIX[1]

[1] Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB),
Lise-Meitner-Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Here, we report on our approach to establish a durable, rigid connection between the Aquarius beamline at synchrotron source Bessy II and its digital counterpart build in the simulation software Ray-UI [1]. While simulations play a crucial role in the instrument design as a digital precursor of the real-world object and contain a comprehensive description of the setup, usually the digital representation is neglected once the real instrument is fully commissioned.

To preserve the symbiosis of simulated and real-world instrument beyond commissioning and approach the digital twin concept we combine the two worlds at the NeXus file level [2]. For this purpose, the instrument section of the NeXus file is enriched by detailed simulation parameters where the current state of the instrument is reflected by including real motor positions, e. g. to incorporate the actual aperture of a slit system. As a result, on one hand, the enriched instrument description increases the reusability of experimental data in sense of the FAIR principles [3] and, on the other hand, allows to perform simulations of a measurement from the NeXus file, ready to be exploited by machine-learning techniques, e. g. for predictive maintenance.

The realization serves as a prototype for a more general implementation and would be straightforward applicable to neutron instruments using the NeXus data format.

[1] P. Baumgärtel, P. Grundmann, T. Zeschke, A. Erko, J. Viefhaus, F. Schäfers, and H. Schirmacher, RAY-UI: New Features and Extensions, AIP Con. Proc. 2054, 060034 (2019).

[2] https://manual.nexusformat.org/index.html

[3] Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al*. The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3,** 160018 (2016). https://doi.org/10.1038/sdata.2016.18

E-mail of the corresponding author: gerrit.guenther@helmholtz-berlin.de

Wednesday, October 12th 2022, 09:50-10:10

DAPHNE4NFDI – towards FAIR and sustainable neutron and photon data

Astrid SCHNEIDEWIND[1], Anton BARTY[2]

[1]*JCNS at MLZ, Forschungszentrum Jülich*
[2]*Deutsches Elektronen-Synchrotron DESY*

DAPHNE4NFDI is a DFG-funded project that brings together users and facilities in photon and neutron (PaN) research to improve data management issues. The German National Research Data Infrastructure initiative (NFDI) aims to ensure, in a systematic manner, that the valuable data generated by German scientists and researchers becomes FAIR (Findable, Accessible, Interoperable and Reusable). In the case of PaN experiments and data, DAPHNE4NFDI is imbedded in the European PaN landscape, meaning that it can build upon and sustain the results hitherto obtained by the PaNOSC and ExPaNDS projects.

The DAPHNE consortium itself is organized along the PaN data workflow by task areas, with more than eighty individual participating scientists from several universities and research centers, covering a large variety of scientific fields. To demonstrate the benefits of FAIR data to the scientific community 11 use cases (pilot projects), dealing with different topics, have started defining metadata for their particular method, testing electronic lab books (ELNs), specifying needs and wishes for reference data bases and (meta)data catalogues. Their results are continually discussed in and between the task areas to find a suitable variety of tools and standards for the community.

At the facilities, (meta)data infrastructures are currently either installed or under development. On the other hand, the developed tools and standards must be user friendly as well as suitable for the desired application, which is why the interaction with scientists within the PaN community is now needed. DAPHNE4NFDI emphasizes the development of software catalogues, and software supply, as well striving to make the data AI-friendly.

Initial results are currently coming now, as catalogues and ELNs are being tested, metadata is being classified, and educational initiatives are being planned. This outcome is presented in the context of progress within NFDI and related developments.

E-mail of the corresponding author: a.schneidewind@fz-juelich.de

Wednesday, October 12th 2022, 10:10-10:30

SampleDB: a web-based electronic lab notebook with a focus on sample and measurement metadata

Florian RHIEM[1]

[1]Forschungszentrum Jülich, PGI/JCNS-TA, Jülich, Germany

Research data management in accordance with the FAIR principles of making data findable, accessible, interoperable and reusable[1] is an important part of good scientific practice. While traditional lab notebooks are very useful, electronic lab notebooks can make it much easier to store research data, metadata in particular, in a way following these principles. However, information is not findable or interoperable simply because it was stored electronically, e.g. as rich text content, and especially flexible metadata that varies between instruments and processes can be difficult to store in a way that it is machine-readable and can actually be searched and found.

SampleDB is a web-based electronic lab notebook with a focus on sample and measurement metadata. It uses a JSON-based schema language to define the flexible metadata that is generated during processes, such as performing an experiment or running a simulation, to validate the information provided via a web-based user interface or an API, and to provide a search function that supports complex expressions and features such as automated unit conversion. Scientists can share data between SampleDB instances, or export them to other systems such as Dataverse, SciCat, and electronic lab notebooks supporting the .eln file format.

In this presentation, we will introduce the core concepts of SampleDB, its schema system and features such as automation via its web API, data export and JupyterHub integration, which can facilitate modern research data management workflows.

[1] M. Wilkinson et al. Sci Data 3, 160018 (2016). DOI: 10.1038/sdata.2016.18

E-mail of the corresponding author: f.rhiem@fz-juelich.de

Wednesday, October 12th 2022, 11:00-11:30

Towards real-time analysis and structural control using in-situ characterization of thin film processing

Fabian ELLER[1], Meike KUHN[1], Christopher GREVE, **Eva M. HERZIG[1]**

[1]University of Bayreuth, Dynamics and Structure Formation – Herzig Group, Bayreuth, Germany

Solution processed thin films are widely used in organic and hybrid electronics. The involved novel materials can have conducting or semi-conducting properties. However, the nanostructure and -morphology of these neat and blended materials are decisive for the resulting function. It is therefore highly desirable to control the molecular arrangement within such thin films. Using examples from organic and hybrid solar cells we attempt to control structural properties by exploiting in-situ characterization using real-time analysis. This way we want to move from the characterization of processing [1,2] towards controlling structural properties in such materials [3,4].

We show the different x-ray and visible light based methods available for in-situ characterization within our laboratory. Furthermore, we give insights into the challenges faced by experimentalists dealing with multiple data sets from several instruments to shift towards structural control.

[1] C. Schötz, C. Greve et al, *Adv. Optical Mater.* **9**, 21, 2101161 (2021).

[2] S. Pröller et al, *Adv. Energy Mater* **6**, 1501580 (2016).

[3] F. Eller et al, *to be submitted*

[4] S. Pröller, et al *ACS Appl. Mater. & Interf.* **12** (5), 5219 (2020).

E-mail of the corresponding author: eva.herzig@uni-bayreuth.de

Wednesday, October 12th 2022, 11:30-11:50

The nSoft autonomous formulation laboratory: X-ray and neutron scattering for industrial formulation discovery

Tyler MARTIN[1], Peter BEAUCAGE[1]

[1]National Institute of Standards and Technology, Gaithersburg Maryland, USA

While scattering methods (SAXS, SANS, WAXS) are workhorse techniques for characterizing model macromolecular formulations, they have not been widely used to characterize real products, largely because the large number of components (10-100) often precludes rational mapping between component fractions, structure, and product stability. Multimodal characterization and machine learning (ML) tools promise to greatly reduce the expense of exploring the stability boundaries of a particular, desirable phase in highly multicomponent products. Here we describe the development of the Autonomous Formulation Laboratory, a highly adaptable platform capable of autonomously synthesizing and characterizing liquid mixtures with varying composition and chemistry using x-ray and neutron scattering in addition to a suite of secondary measurements such as optical imaging, UV-vis-NIR and capillary rheometry. We will highlight our efforts in deploying an active-learning agent which controls all aspects of the AFL including sample composition choice, sample preparation, characterization, and analysis. Using our agent, we can resolve phase boundaries at high resolution with as much as a 95% reduction in measurement time compared to a naïve grid search.

E-mail of the corresponding author: tyler.martin@nist.gov

Wednesday, October 12th 2022, 11:50-12:10

High accuracy neutron diffraction measurement using an industrial robot system at the STRESS-SPEC instrument

Martin LANDESBERGER[1], Lijiu WANG[1], **Michael HOFMANN[1]**, Weimin GAN[1], Oguz KEDILIOGLU[2], Heinz-Günter BROCKMEIER[3]

[1] Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich (TUM), Lichtenbergstr. 1, 85748 Garching, Germany
[2] Institute for Factory Automation and Production Systems (FAPS), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Egerlandstr. 7, 91058 Erlangen, Germany
[3] Institut für Werkstoffkunde und Werkstofftechnik, Clausthal University of Technology Agricolastr. 6, 38678 Clausthal-Zellerfeld, Germany

The Heinz Maier-Leibnitz Zentrum (MLZ) operates at Germany's sole neutron source FRM II the diffractometer STRESS-SPEC 31ichael31d for fast strain mapping and texture analyses. The STRESS-SPEC group was the first to pioneer sample handling and positioning via industrial robots at neutron diffractometers [1, 2]. However, the current robot is limited in its use due to insufficient absolute positioning accuracy of up to ± 0.5 mm in some cases. Usually, an absolute positioning accuracy of 10% of the smallest gauge volume size – which in case of modern neutron diffractometers is in the order of 1×1×1 mm^3 – is necessary to allow accurate strain tensor determination and correct centering of local texture measurements. The original robot setup at the neutron diffractometer STRESS-SPEC has therefore been upgraded to a high accuracy positioning/metrology system. We will give a short introduction on the complete measurement process chain for the new robot environment. To achieve a spatial accuracy of 50 μm or better during measurement of the full strain tensor, the sample position is tracked by an optical metrology system and actively corrected, which we will show in detail.

[1] H.-G. Brokmeier et al., Mater. Sci. For. **652** (2010) pp. 197–201.

[2] C. Randau et al., Nucl. Instr. Meth. A: 794 (2015) pp. 67–75.

[3] V. Luzin, N. Hoye, Mater. Res. Proc. 2 (2017) pp. 497–502.

E-mail of the corresponding author: michael.hofmann@frm2.tum.de

Wednesday, October 12th 2022, 12:10-12:30

Adaptive data acquisition at the hot single crystal diffractometer HeiDi at MLZ: What do we have and what will we need in the future?

Martin MEVEN[1,2], Piotr FABRYKIEWICZ[1,2], Andrzej GRZECHNIK[2], Wolfgang LUBERSTETTER[1,2], Georg BRANDL[2], Jens KRÜGER[3], Mirijam ZOBEL[1]

[1]Institute of Crystallography, RWTH Aachen University, Aachen, Germany

[2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany

[3]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany

The single crystal neutron diffractometer HeiDi at the hot source of FRM II supports various grand challenges in research as well as method developments since almost two decades. Its key features are fast and high quality Bragg data collections up to very large Q (> 20/Å for λ=0.56Å), within a broad temperature range (2K < *T* < 1300K) and, since 2019, also high pressure experiments (< 10 Gpa). The continuous optimization and extension of HeiDi's hardware are essential prerequisites for successful user operation.

The full exploitation of these options and the secure support of 24h/7d operation requires a very flexible and autonomous software for device control and data acquisition. Accordingly, the HeiDi software already contains many routines, which can be related to "machine learning" as they allow during a running experiment to determine and to adopt automatically the best possible parameters for sample centering, sample orientation and reflection collection or to avoid collisions and shading. Other routines allow to simulate the expected beam time for data collection dependent on sample features like space group or profile widths.

Our presentation shows the existing possibilities as well as our future ideas: We plan to port our software and its adaptive features to a NICOS based control software. Also, we want to expand typical single crystal related multiparameter measurement options like T-dependent intensity measurements, multidimensional Q-scans or the extraction of weak reflection intensities (e.g. with PSD). The last topic requires the integration of software for reading out or analyzing PSD data (e.g. NSX-Tools or MANTID). In addition, we wish to prepare our instrument to new challenges like PDF studies up to high Q and use of related software tools.

[1] M. Meven et al. (MLZ); Journal of large-scale research facilities **1** A7, (2015).
[2] A. Grzechnik et al.; J. Appl. Cryst. **53(1)**, 1 – 6; (2020).
[3] F. Magro et al.; J. Appl. Cryst. **54**, 822-829; (2021).

E-mail of the corresponding author: martin.meven@frm2.tum.de

Wednesday, October 12th 2022, 13:40-14:10

Maximising information gain and optimizing experimental design for neutron reflectivity

J. H. Durant; L. Wilkins; **J. F. K. COOPER**

[1]ISIS neutron and Muon Source, Harwell Campus, Didcot, OX11 0QX, UK

Many of us will perform a neutron experiment and be content if the data which we obtain at the end of it "looks nice", by whatever metric we have from experience. This experience has often caused us to develop rules of thumb, where we know that measuring, for example, 2 hours on this sample will give nice looking data from which we will probably be able to extract the material properties we want. Obviously during an experiment, we want to be able to measure as many samples as possible. However, the fear of not measuring long enough, and then not being able to extract your material parameters, can often lead us to over-count samples.

In this talk I present a recently developed formalism[1,2] based on the Fisher information, which enables us to determine the amount of information that a neutron dataset contains about the material parameters that we wish to extract. The formalism is general to all Poisson/count based techniques, but I present the framework applied to neutron reflectivity. I will show how being able to relate the number of neutron counts to our knowledge about material parameters can inform us not only how long we need to measure a sample for, but also how to perform a better experiment in the first place.

[1] J.H. Durant, L. Wilkins, K. Butler, J.F.K. Cooper, J. Appl. Crystal. **54** (2021).

[2] J.H. Durant, L. Wilkins, J.F.K. Cooper, J. Appl. Crystal. **55** (2022).

E-mail of the corresponding author: Jos.Cooper@STFC.ac.uk

Wednesday, October 12th 2022, 14:10-14:40

Bringing Machine Learning to Beamline

Alexander HEXEMER[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, USA

The scientific user facilities (SUF) of the Department of Energy (DOE) are some of the world's largest producers of scientific data from experiments, modeling, and simulation. The data generated spans multidisciplinary sciences covering multi-faceted and complex interactions that require domain expertise to decipher intricate relationships within natural phenomena. There is tremendous potential in coordinating complex data analysis. This can aid in building, optimizing the use of experimental facilities, increasing transparency, and accelerating discovery. As it is now, each experimentalist gathers data and scientific insight into a small part of complex physical phenomena. Restricted to limited pools of scientific data or summarized content of formal publications, intricate relationships are lost. Machine learning and artificial intelligence promise a ready-to-use approach to solving complex problems and accelerating data analysis and knowledge extraction. Driven by industry, machine learning frameworks are being developed rapidly. However, the applications in science and, in particular, the world of scientific user facilities is less evolved. The threshold of developing, training, and testing machine learning models is still very steep and requires significant time commitment by beamline scientists. MLExchange targets this threshold with the development and deployment of easy-to-use solutions that target science performed at SUFs. We will present our first developments in labeling, segmentation, and XRD.

E-mail of the corresponding author: ahexemer@lbl.gov

Wednesday, October 12th 2022, 14:40-15:00

Automated software and advanced tools for treating small-angle scattering and reflectivity data from bio-molecular structures

Alexandros KOUTSIOUMPAS[1]

[1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ),
Forschungszentrum Jülich GmbH, Lichtenbergstrasse 1, 85748 Garching, Germany

Small-angle scattering and reflectivity of neutrons and x-rays are routinely used by numerous groups worldwide for the study of the structure of biological molecules in the bulk and close to interfaces. Notable examples include a) low-resolution conformational studies of proteins and nucleic acids in solution and b) the determination of accurate density profiles of supported phospholipid membranes close to hydrophilic substrates.

In the past few years we have introduced several software tools that offer new capabilities in relation to the treating experimental data from the above mentioned systems. In this contribution we review three examples:

- DENFERT webserver [1,2,3] offers a simplified and fully automatic way for recovering the low-resolution structure of biological molecules from solution SANS and SAXS.
- DIONYSIA program [4] may provide a model-free interfacial structure from multi-contrast reflectivity data within the limits of finite spatial resolution.
- ANAKLASIS open source package [5,6] offers unique capabilities in relation to statistically accurate fits of reflectivity data by also simplifying elaborate model definition.

By showcasing past and current applications of all these software packages, we focus our discussion on their potential in attracting scientists from different disciplines into performing research in large scale neutron and x-ray facilities.

[1] A. Koutsioubas & J. Pérez, J. Appl. Cryst. **46**, 1884 (2013).

[2] A. Koutsioubas, S. Jaksch & J.Pérez, J. Appl. Cryst. **49**, 690 (2016).

[3] https://alexandros-koutsioumpas.github.io/Denfert/

[4] A. Koutsioubas, J. Appl. Cryst. **52**, 538 (2019).

[5] A. Koutsioubas, J. Appl. Cryst. **54**, 1857 (2021).

[6] https://github.com/alexandros-koutsioumpas/anaklasis

E-mail of the corresponding author: a.koutsioumpas@fz-juelich.de

Wednesday, October 12th 2022, 15:00-15:20

Storage and Infrastructure for Big Data and AI

Michael LINKE, Fabian SCHÜLZLE, Nicolai SCHMID, Michael DRÜING

Advanced UniByte GmbH

Advanced UniByte (AU) is an expert for future-oriented and flexible IT infrastructure, as well as services in the area of storage, compute, virtualization, network and backup. They are also experts for cloud-/managed-services and SAP HANA.

https://www.au.de/

Wednesday, October 12th 2022, 16:00-16:30

Fast Calculation of Scattering Patterns Using Hypergeometric Function Algorithms

Michael WAGENER[1], **Stephan FÖRSTER[1]**

[1] JCNS, Forschungszentrum Jülich, Jülich, Germany

The scattering of light, X-rays, electrons or neutrons by matter is used widespread for structural characterization from atomic to macroscopic length scales. With the advent of high-brilliance beam sources and the development fast, large area pixelated detectors, scattering patterns are now acquired at unprecedented frame rates and frame sizes. The slow analysis of these scattering patterns has evolved into a severe bottleneck retarding scientific insight.

Here, we present an algorithm that is based on the use of hypergeometric functions to rapidly compute 1D- and 2D-scattering data. Hypergeometric functions provide a simple mathematical description of geometrical objects, have analytical Fourier transforms, and can be rapidly computed via series and asymptotic expansions with recursive coefficients. Compared to numerical integration schemes we observe gains in computation speed of $> 10^5$. The algorithms can be efficiently implemented in GPUs for further acceleration.

The algorithm provides the necessary computational speed to calculate scattering patterns on timescales required for real-time experiment feedback, the analysis of large volumes of scattering data, and for the generation of training data sets for machine learning. It enables the computation of 2D scattering patterns at > 1 fps even for current 4k pixel detectors.

E-mail of the corresponding author: s.foerster@fz-juelich.de

Wednesday, October 12th 2022, 16:30-16:50

Classification of Small-Angle Scattering Patterns Using Machine Learning on Transformed 2D-Data

Michael WAGENER[1], **Marina GANEVA**[1], Stephan FÖRSTER[1]

[1] JCNS, Forschungszentrum Jülich, Jülich, Germany

X-ray and neutron scattering are widely used powerful techniques for probing the physical structure of materials at the molecular and supramolecular scale. With the simultaneous advent of high-speed detectors, previously unimaginable time-resolved *in situ* and high throughput photon and neutron experiments have become possible, with the subsequent explosion of data volumes. Data analysis is becoming the most serious bottleneck on the way from experiment to scientific insight and final publication. We aim to provide rapid machine learning-based data classification to (i) guide decisions during the course of an experiment and to (ii) guide users as to which models are most appropriate for subsequent data analysis.

We developed a methodology where the small-angle scattering patterns or 2D detector data are first transformed from (q_x,q_y) into (r,ϕ)-coordinates to become independent of the specific beam position on the detector and the specific detector pixel array format. The subsequent Fourier transform transforms the data from (r,ϕ)- to a real-space representation in Carthesian (x,y) coordinates. This makes use of Friedel's law and the Fourier shift theorem for a reduced presentation of the data. It is thus possible to operate with one training set for different instruments and different detectors. We used a broad range of experimental and simulated 2D-scattering data for spheres, ellipsoids, isotropic and oriented cylinders, as well as ordered lattice structures consisting of spheres, cylinders or lamellae of different degree of positional and orientational order and polydispersity.

In the present work we compare performance of various classifiers, including decision trees, random forest, as well as probabilistic classification using variational inference neural networks. We show, that the transformed data can be better classified compared to the original 2D-detector data, enabling a reliable fast classification of scattering patterns with the possibility for a subsequent automatized data analysis with the selected models.

E-mail of the corresponding author: m.ganeva@fz-juelich.de

Wednesday, October 12th 2022, 16:50-17:10

Real-time data processing for serial X-ray crystallography

Thomas WHITE[1], Tim SCHOOF[1], Sergey YAKUBOV[1], Aleksandra TOLSTIKOVA[1], Valerio MARIANI[3], Alessandra HENKEL[2], Bjarne KLOPPROGGE[2], Andreas PRESTER[2], Stijn DE GRAAF[2], Marina GALCHENKOVA[2], Oleksandr YEFANOV[2], Jan MEYER[1], Guillaume POMPIDOR[1], Juergen HANNAPPEL[1], Dominik OBERTHUER[2], Johanna HAKANPÄÄ[1], Martin GASTHUBER[1], Anton BARTY[1]

[1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

[2]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

[3]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, USA

We have implemented a system for fully real-time data processing during a serial X-ray diffraction experiment, with (in principle) no need to store image data on disk. Using the CrystFEL software [1] in combination with the ASAP::O data framework, frames from a 16 megapixel Dectris EIGER2 X detector were searched for peaks, indexed and integrated at the maximum full-frame readout speed of 133 frames per second. The pipeline produced un-merged Bragg reflection intensity measurements which could be directly scaled and merged in order to solve the structure.

With a careful choice of parameters for data processing, only 32 CPU cores were needed to keep up with the data even when 40% (a relatively large fraction) of frames were not rapidly rejected by an initial “hit finding” step.

Real-time data processing offers many advantages, not least the possibility of reducing or eliminating the need for bulk data storage after the experiment. But are we ready to make the required changes to our established workflows? This presentation will discuss the impact on the way we perform experiments at large-scale facilities.

[1] T. A. White et al., J. Appl. Cryst., 49, p680 (2016).

E-mail of the corresponding author: thomas.white@desy.de

FAIR data principles and reflectivity analysis using GenX 3

Artur GLAVIC[1]

[1]Laboratory for Neutron and Muon Instrumentation,
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Experiments that are (at least in principle) repeatable and transparent data treatment are the corner stones of the scientific method. The quality of future research depends on these aspects to not only be considered when performing such experiments and describing them in peer reviewed publications but also when storing the associated data and analysis results in a manner that makes it not only possible but practical to work with for independent scientists. For this reason, the data should be Findable, Accessible, Interoperable and Reusable (FAIR [1]). When well implemented the FAIR principles not only allow others to repeat or re-analyze previous results but can also aid automatized analysis approaches as, for example, the training of AI systems.

In (neutron) reflectometry it was realized by the community that there is a need to improve the current practice in storing and reporting reduced data and analysis results. The Open Reflectometry Standards Organization (ORSO) [2] was founded by experts from various research institutes and universities to work towards a standardized data format, evaluation of analysis software, a common model description language and related goals. The first version of a standard ASCII based data format with pre-defined header fields has recently been released on the ORSO website.

I will present recent developments of the GenX reflectivity analysis software [3] that implement this ORSO standard. Together with the ORSO SLD database and a simple model description language, that is still in development, it is possible to quickly create a sample model automatically and thus aid the data analysis workflow. The resulting fits can be analyzed using statistical methods and exported in the ORSO format with header information that directly allows a recreation of the model. All metadata from the original file is preserved. For related datasets from measured sequences, it is now possible to apply batch fits and evaluate the ORSO header information to quickly display the relationship of a fit parameter to experimental values like temperature of magnetic field.

[1] M. Wilkinson, et al., Scientific Data, **3**, 160018 (2016)
[2] T. Arnold, A. Glavic, J. F. K. Cooper, Neutron News, **32**, 7-8 (2021)
https://www.reflectometry.org/
[3] A. Glavic and M. Björck, J. Appl. Cryst., **55**, https://doi.org/10.1107/S1600576722006653

E-mail of the corresponding author: Artur.glavic@psi.ch

Automated sample loading using Panda cobot from Franka Emika

Konstantin KHOLOSTOV, Klaus Bussmann, Georg Brandl, Artem Feoktystov

Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH
Lichtenbergstraße 1, 85748 Garching, Germany

Robots and cobots (collaborative robots) were designed to change manufacturing and production processes at factories. Typical application of an industrial robot would be to replace a human on repetitive tasks, which involve endurance, speed, and precision. Industrial robots usually operate in environments isolated from human contact. Instead, cobots are designed to provide human robot interaction within a shared space: they are build out of lightweight materials with rounded edges, demonstrate human-like speed and force, and are equipped with torque sensors to handle collisions.

Neutron hall is an environment with extra safety protocols due to its radiation sources. One of the strategies to mitigate the risk of radiation exposure would be to reduce presence of workers in the hall to minimal times if not to avoid completely. For that certain operations could be automated and executed in a given time by a robot.

In this work we demonstrate an automated system for sample loading to one of the instruments, located in the neutron hall of Heinz Maier-Leibnitz Zentrum. This system is built using Panda cobot from Franka Emika Gmbh. The control software is written in C++ [1] and is integrated into TANGO network at MLZ.

[1] https://forge.frm2.tum.de/review/plugins/gitiles/jcns/tango/franka/+/refs/heads/master

E-mail of the corresponding author: k.kholostov@fz-juelich.de

Data acquisition routines on the polarized neutron single crystal diffractometer POLI at MLZ

Jianhui XU[1,2], Henrik THOMA[1,2], Vladimir HUTANU[3], Wolfgang LUBERSTETTER[1,2], Martin MEVEN[1,2], Georg BRANDL[2], Georg ROTH[1], Mirijam ZOBEL[1]

[1]Institute of Crystallography, RWTH Aachen University, Aachen, Germany

[2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Germany

[3]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany

Polarized neutron diffraction is a powerful tool for studying condensed matter physics and probing the spin and orbital properties of unpaired electrons. It allows to unambiguously determine complex magnetic correlations and small ordered moments, separate magnetic and nuclear contributions, and study spin-orbital entangled states by mapping out the atomic magnetization density at the unit cell level. POLI is a polarized neutron single crystal diffractometer built on the hot neutron source at MLZ [1].

Currently, three standard setups are implemented on POLI: 1) zero-field spherical neutron polarimetry using third generation CRYOPAD; 2) polarized neutron diffraction in magnetic fields (Flipping-Ratio method); 3) non-polarized diffraction under various special conditions [2-4]. The three setups are quite different in the data collection process and to take advantage of the neutron polarization, precise and frequent manipulations and analyses of neutron polarization are required. Therefore, it is complicated and time-consuming to obtain high quality data, especially considering the point detector and various sample environments currently used on POLI. However, owning to the flexibility of the NICOS instrument control system, we develop different measurement routines in the Python language for the three different setups to facilitate performing experiments on POLI which will be present here.

[1] V. Hutanu, Journal of large-scale research facilities, **1**, A16 (2015).

[2] H. Thoma, H. Deng, G. Roth, and V. Hutanu, Journal of Physics: Conference Series **1316**, 012016 (2019).

[3] V. Hutanu et al., IEEE Transactions on Magnetics **58**, no. 2, pp. 1-5, (2022).

[4] V. Hutanu, et al., Review of Scientific Instruments **87**, (2016).

E-mail of the corresponding author: jianhui.xu@tum.frm2.de

Real-time data processing for serial X-ray crystallography

Thomas WHITE[1], Tim SCHOOF[1], Sergey YAKUBOV[1], Aleksandra TOLSTIKOVA[1], Valerio MARIANI[3], Alessandra HENKEL[2], Bjarne KLOPPROGGE[2], Andreas PRESTER[2], Stijn DE GRAAF[2], Marina GALCHENKOVA[2], Oleksandr YEFANOV[2], Jan MEYER[1], Guillaume POMPIDOR[1], Juergen HANNAPPEL[1], Dominik OBERTHUER[2], Johanna HAKANPÄÄ[1], Martin GASTHUBER[1], Anton BARTY[1]

[1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

[2]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

[3]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, USA

We have implemented a system for fully real-time data processing during a serial X-ray diffraction experiment, with (in principle) no need to store image data on disk. Using the CrystFEL software [1] in combination with the ASAP::O data framework, frames from a 16 megapixel Dectris EIGER2 X detector were searched for peaks, indexed and integrated at the maximum full-frame readout speed of 133 frames per second. The pipeline produced un-merged Bragg reflection intensity measurements which could be directly scaled and merged in order to solve the structure.

With a careful choice of parameters for data processing, only 32 CPU cores were needed to keep up with the data even when 40% (a relatively large fraction) of frames were not rapidly rejected by an initial “hit finding” step.

Real-time data processing offers many advantages, not least the possibility of reducing or eliminating the need for bulk data storage after the experiment. But are we ready to make the required changes to our established workflows?

This poster presentation will give an opportunity for further discussion of the issues raised in the oral presentation with the same title.

[1] T. A. White et al., J. Appl. Cryst., 49, p680 (2016).

E-mail of the corresponding author: thomas.white@desy.de

SECoP AND METADATA – THE SAMPLE ENVIRONMENT COMMUNICATION PROTOCOL

Klaus Kiefer[1], **Georg BRANDL[2]**, Niklas Ekström[3], Enrico Faulhaber[4], Thomas Herrmannsdörfer[5], Bastian Klemke[1], Thorsten Kracht[6], Anders Pettersson[3], Lutz Rossa[1], Markus Zolliker[7]

[1]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

[2]Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich, Lichtenbergstraße 1, 85748 Garching, Germany

[3]European Spallation Source, Partikelgatan 2, 224 84 Lund, Sweden

[4]Forschungs-Neutronenquelle Heinz Maier-Leibnitz, Lichtenbergstraße 1, 85748 Garching, Germany

[5]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

[6]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

[7]Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen, Switzerland

The integration of sample environment (SE) equipment in a beam line experiment is a complex challenge both in the physical world and in the digital world. Different experiment control software offer different interfaces for the connection of SE equipment. Therefore, it is time-consuming to integrate new SE or to share SE equipment between facilities.

To tackle this problem, the International Society for Sample Environment (ISSE) developed the Sample Environment Communication Protocol (SECoP) to standardize the communication between instrument control software and SE equipment (see [1] and references therein). SECoP offers, on the one hand, a generalized way to control SE equipment. On the other hand, SECoP holds the possibility to transport SE metadata in a well-defined way.

Using SECoP as a common standard for controlling SE equipment and generating SE metadata will save resources and intrinsically give the opportunity to supply standardized and FAIR data compliant SE metadata. It will also supply a well-defined interface for user-provided SE equipment, for equipment shared by different research facilities and for industry.

In this presentation we will give an overview of the present status of SECoP and the developments within the SECoP@HMC project supported by the Helmholtz Metadata Collaboration.

[1] K. Kiefer, et al. An introduction to SECoP – the sample environment communication protocol. Journal of Neutron Research, **21**(3-4), 181–195 (2020).

E-mail of the corresponding author: g.brandl@fz-juelich.de

Abstracts

Thursday, October 13th 2022

Thursday, October 13th 2022, 09:00-09:30

Online material studies by the Bilbao Crystallographic Server

Mois I. AROYO, Gemma de la Flor Martin[2], Emre S. Tasci[3], J. Manuel Perez-Mato[1], Luis Elcoro[1], Gotzon Madariaga[1]

[1]Physics Department, University of The Basque Country (UPV/EHU), Bilbao, Spain

[2]Institut of Applied Geoscience, Karlsruhe Institute of Technology, Karlsruhe, Germany

[3]Department of Physics Engineering, Hacettepe University, Ankara, Turkey

The *Bilbao Crystallographic Server* (www.cryst.ehu.es) is a free website with access to crystallographic data of space and point groups, magnetic space groups, subperiodic groups, their representations, and group-subgroup relations [1, 2]. A database on incommensurate structures incorporating modulated structures and composites, a magnetic-structure database and a **k**-vector database with Brillouin-zone figures are also available. A wide range of complex solid-state physics and structure-chemistry aspects of materials studies are facilitated by the specialized software provided by the server.

The server offers a set of structure-utility programs including basic tools for crystal-structure transformations or transformations compatible with a specific symmetry reduction. There are online tools for quantitative analysis of similarity of different structure models (helpful also for the recognition of identical or nearly-identical atomic arrangements of different compounds) or the analysis of crystal-structure relationships that are of great utility for the construction of family trees of homeotypic crystal structures. There are tools for systematic studies of phase-transition mechanisms including the evaluation of structural pseudosymmetry which could serve as a powerful method for the prediction of new ferroic materials. Recently implemented computational tools and databases allow the systematic application of symmetry arguments in the study of magnetic structures.

The presentation of the databases and programs offered by the Bilbao Crystallographic Server will be accompanied by case studies illustrating the capacity and efficiency of the online tools in material studies.

[1] M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov & H. Wondratschek. *Z. Kristallog.*,**221**, 15-27 (2006).

[2] M. I. Aroyo, J. M. Perez-Mato, D. Orobengoa, E.T. Tasci, G. De la Flor, A. Kirov. *Bulgarian Chem. Comm.,* **43**(2), 183-197 (2011).

Corresponding author email: mois.aroyo@ehu.es

Thursday, October 13th 2022, 09:30-09:50

Ten years Scientific Computing Group at MLZ - our quest for sustainable data analysis software

Joachim WUTTKE

Forschungszentrum Jülich, JCNZ-MLZ, Garching, Germany

The Scientific Computing Group at MLZ Garching was created in 2012 to develop and maintain software for neutron scattering data reduction and analysis. Ten years later, this is a good occasion to review our achievements and experiences. I will present the software developed so far, and discuss the challenges of making the development of research software sustainable.

[1] J. Wuttke, S. Cottrell, M. A. Gonzalez, A. Kaestner, A. Markvardsen, T. H. Rod, P. Rozyczko, G. Vardanyan: Guidelines for collaborative development of sustainable data treatment software. J. Neutron Res. 24, 33-72 (2022).

E-mail of the corresponding author: j.wuttke@fz-juelich.de

Thursday, October 13th 2022, 09:50-10:10

The new versions 3.5 and 4.0 of the instrument simulation program VITESS

Klaus LIEUTENANT[1], Jörg VOIGT[1], Zhanwen MA[1], Fabian BEULE[2], Stefan MATTAUCH[3], Jingjing LI[2], Egor VEZHLEV[2]

[1]Forschungszentrum Jülich, JCNS-2 / PGI-4, 52425 Jülich, Germany

[2]Forschungszentrum Jülich, JCNS, 52425 Jülich, Germany

[3]Forschungszentrum Jülich, JCNS-4, 85748 Garching, Germany

The new VITESS versions 3.5 and 4.0 have recently been finished. VITESS 4 is designed to be used for virtual experiments, e.g. at MLZ. The instruments are stored as yaml files, which enables changing the instrument parameters from NICOS (as in a real experiment). For maintenance and performance reasons, the new GUI is written in Qt and the monitor output will be visualized using the FZJ program GR. Version 4.0 will not have the complete set of modules, but only those found in many instruments, altogether 36 out of 58. Additionally, the use of parameters from files is reduced. It is under test now for virtual experiments at the neutron reflectometer MARIA at MLZ in Garching.

As it will take time to get VITESS 4 complete and faultless, version 3 will still be needed for some time. VITESS 3.5 contains several new features that are needed for instrument simulations for the HBS, e.g. a source module for HBS and a rotating monochromator. It also contains already many improvements realized for the virtual experiments like additional features for the reflectometer sample and monitor update during the run. The HBS source is also available in McStas. Next year, version 3.6 will be written with the main new feature to save instruments, stored under version 3, in the new format using yaml files. Then, all missing modules will be added to version 4 and released as version 4.1.

We will present the main new features of version 3.5 and 4.0 and also show how to simulate the HBS source, both in VITESS and in McStas.

E-mail of the corresponding author: k.lieutenant@fz-juelich.de

Thursday, October 13th 2022, 10:10-10:30

Particle transport simulations for the design of the HBS Target-Moderator-Reflector assembly

Jingjing LI[1], Paul ZAKALEK[1], Ulrich RÜCKER[1], Eric MAUERHOFER[1], Norberto SCHMIDT[1], Klaus LIEUTENANT[1], **Egor VEZHLEV[2]**, Jörg VOIGT[1], Thomas GUTBERLET[1], and Thomas BRÜCKEL[1]

[1]Forschungszentrum Jülich GmbH, JCNS, Jülich, Germany

[2]Forschungszentrum Jülich GmbH, JCNS at MLZ, Garching, Germany

The concept for the accelerator-driven High Brilliance neutron Source (HBS) is currently being in active design phase. The overall key optimization parameters in the design of this novel neutron source are: maximum brilliance at the instruments, rather compact dimensions, flexibility and cost efficiency. In this respect thorough and detailed simulations by means of particle transport codes are of a great importance. The simulated performance parameters, like neutron yield from the target, neutron fluxes at the cold and thermal moderators, achievable brilliance at the extraction channels give a rather promising outlook for the performance of future instruments to be built at the HBS neutron source. We are going to present the latest achievements of the work of the HBS simulation group regarding optimization of the Target-Moderator-Reflector (TMR) assembly. In addition, our current work on combining the results of these simulations with the design and development of the HBS instrument suite will be discussed.

E-mail of the corresponding author: e.vezhlev@fz-juelich.de

Thursday, October 13th 2022, 11:00-11:30

Quantifying structural ambiguity from polydisperse parameter inversion in small-angle scattering

Kuangdai LENG[1], Stephen KING[2], Tim SNOW[3], Sarah ROGERS[2], Anders MARKVARDSEN[2], Satheesh MAHESWARAN[3], Jeyan THIYAGALINGAM[1]

[1]Scientific Computing Department, STFC, Rutherford Appleton Laboratory, Didcot OX11 0QX, UK

[2]ISIS Neutron and Muon Source, STFC, Rutherford Appleton Laboratory, Didcot OX11 0QX, UK

[3]Diamond Light Source, Rutherford Appleton Laboratory, Didcot OX11 0QX, UK

The inverse problem in small-angle scattering (SAS) can be summarised as finding the maximum likelihood estimation (MLE) of the polydisperse distributions of model parameters (such as size and orientation of inclusions), given the scattering intensity (either a curve or an image) observed from a SAS experiment. We have developed a new model- and form-free method to solve this inverse problem for general multi-parameter models [1]. Equipped with a special data scaling algorithm for accuracy enhancement, our method has reached an unprecedented precision for the minimisation of the fitting error; e.g., our benchmark problem shows that our χ^2-error is 10^9~10^{12} smaller than those obtained by the previous methods.

Such high accuracy reveals that SAS inversion is subject to a high degree of non-uniqueness of solution or *structural ambiguity*. It means that very different parameter distributions can predict identical scattering intensities as measured in reference to data uncertainty. We will visualise and quantify such structural ambiguity from both theoretical and numerical perspectives based on size distribution inversion. Structural ambiguity is an inherent limit of SAS data analysis, which should be understood and handled properly.

Though a solution closer to the MLE (giving a smaller fitting error) may not necessarily be plausible due to overfitting, they should be provided by an inverse method as a candidate. However, due to issues arising from insufficient accuracy, some of the previous methods can lead to underfitting solutions, usually smooth and dispersive, which may be far away from the ground truth. In contrast, our method can provide a series of solutions fitting the data, covering the transition regime from underfitting to overfitting. This can enable the users to select the most appropriate solution meeting their physical or empirical constraints, providing a safe way to address the issues around structural ambiguity.

[1] K. Leng, S. King, T. Snow, et al., Journal of Applied Crystallography, **in press** (2022).

E-mail of the corresponding author: kuangdai.leng@stfc.ac.uk

Thursday, October 13th 2022, 11:30-11:50

Materials informatics approach on neutron scattering data for the development of anion exchange membranes used for next-generation energy devices

Yue ZHAO[1], **Aurel RADULESCU[2]**, Yasunari MAEKAWA[1], Peter MÜLLER-BUSCHBAUM[3]

[1]Takasaki Advanced Radiation Research Institute, National Institutes for Quantum and Radiological Science and Technology (QST), Takasaki, Gunma, 370-1292, Japan

[2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), 85748 Garching, Germany

[3]Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München and Heinz Maier-Leibnitz Zentrum (MLZ), 85748 Garching, Germany

We aim to apply "materials informatics" (MI) for the development of high-performance anion-exchange membranes (AEM), which may be applied to next generation energy devices, such as non-platinum fuel cell hybrid vehicles and all solid secondary batteries. Currently, there are two major obstacles to using MI for such systems: the unclear higher-order (hierarchical) structure/function relationship of AEM and the lack of a comprehensive structural database under various practical temperature/humidity conditions. We plan to use scattering and simulation methods, in particular the unique CV-SANS (Contrast-Variation Small Angle Neutron Scattering) technique with precise Partial Scattering Function (PSF) analysis, to obtain an accurate structure of each component in real AEMs under practical operating conditions and also to target various AEMs prepared by Radiation Graft Polymerization (RGP), which allows to impart new functionality to graft polymers while maintaining the mechanical and thermal properties of base polymers. A structural dataset will be defined through CV-SANS, microscopy and simulations, and we aim to create new optimized AEM through machine learning algorithms using this database. In our recent studies on hydrated proton exchange membrane (PEM) systems we introduce CV method to conventional SANS measurements to give multiple profiles for one sample under one operation condition (*i.e.* multiple equations), which are necessary for unique PSF analysis to determine precise structure of each component [1, 2]. Examples of PSF analysis of CV-SANS data and the plans on using MI for next generation AEMs will be reported.

[1] Y. Zhao et al., Macromolecules **54**, 4128 (2021).

[2] Y. Zhao et al., Macromolecules in press (2022).

E-mail of the corresponding authors: a.radulescu@fz-juelich.de; zhao.yue@qst.go.jp

VITESS simulation and virtual experiment of the neutron diffractometer for small samples at the High Brilliance Neutron Source

Zahnwen MA[1], Klaus LIEUTENANT[1], Jörg VOIGT[1], Tobias E. SCHRADER[2], Thomas GUTBERLET[1], Thomas BRÜCKEL[1]

[1] Forschungszentrum Jülich, Jülich Centre for Neutron Science, 52425 Jülich, Germany
[2] Forschungszentrum Jülich, Jülich Centre for Neutron Science at Heinz Maier-Leibnitz-Zentrum (MLZ), Lichtenbergstr. 1, 85748 Garching, Germany

For the sustainable development of the neutron community in Europe and Germany, the High Brilliance Neutron Source (HBS) has been proposed at the Julich Center for Neutron Science (JCNS) [1]. The accelerator, target, and moderators of HBS have been optimized to achieve a high moderator surface peak brilliance comparable to a medium flux reactor source or medium power spallation sources [2]. The instruments are optimized by Monte-Carlo simulations to make full use of the high brilliance and high flexibility of the HBS.

The low dimensional moderators of HBS are well suited for the investigation of small samples [3]. For example, in neutron macromolecular crystallography, typical sample volumes reach from 0.01 mm^3 to 1 mm^3 [4]. As the scattered signal is small, special care must be taken to keep the instrumental background extremely low. In this work, the design progress of a macromolecular diffractometer, including the optimization of the instrument and the evaluation of the virtual experiments, will be presented. By tailoring a small, appropriately collimated beam far upstream of the sample position, we can obtain a low background tunable neutron beam at a 1 mm^2 sample with a flux comparable to the existing instruments at spallation neutron sources or reactor sources.

[1] T. Gutberlet *et al*., "The Jülich high brilliance neutron source project – Improving access to neutrons," *Phys. B Condens. Matter*, **vol. 570**, no. December 2017, pp. 345–348, (2019).

[2] T. Brückel *et al*., "Conceptual Design Report Jülich High Brilliance Neutron Source (HBS)," Forschungszentrum Jülich GmbH, (2020).

[3] T. Cronert *et al*., "High brilliant thermal and cold moderator for the HBS neutron source project Jülich," *J. Phys. Conf. Ser*., **vol. 746**, no. 1, (2016).

[4] M. P. Blakeley and A. D. Podjarny, "Neutron macromolecular crystallography," *Emerg. Top. Life Sci*., **vol. 2**, no. 1, pp. 39–55, (2018).

E-mail of the corresponding author: zh.ma@fz-juelich.de

Thursday, October 13th 2022, 12:10-12:30

Leveraging containerization technology for FAIR data management

Georg BRANDL[1], **Christian FELDER**[1], Moritz HANNEMANN[1], Osca MUKIRI[1]

[1]Forschungszentrum Jülich GmbH, JCNS at MLZ, Garching, Germany

The DAPHNE initiative, as part of the German National Research Data Infrastructure (NFDI), is facing the common challenge of coping with the increasing need for unified external data access and analysis solutions of large amounts of data according to the "FAIR" principles. FAIR stands for Findable, Accessible, Interoperable and Reusable and describes the criteria for sustainable usability of research data. In this talk we will showcase the steps from performing an experiment, using a digital twin, to analyse the data in the cloud also known as data analysis as a service, including a live demonstration.

E-mail of the corresponding author: c.felder@fz-juelich.de

Thursday, October 13th 2022, 13:40-14:10

Modernizing SNS Neutron Scattering Instruments with proven Control System tools

Klemen VODOPIVEC[1]

[1]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, USA

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory operates 19 neutron scattering instruments with diverse experimental capabilities and unique sample environments. Instrument staff and scientists are constantly exploring research opportunities and developing new techniques for continuous instrument improvements. This often results in adding new apparatus or software-assisted techniques that need to be integrated into instrument control system, which must be robust and flexible at the same time.

Between 2015 and 2019, most neutron scattering instruments at SNS were converted to EPICS control system and received upgraded experiment planning, complete experiment automation and outperforming data acquisition system. These upgrades allow SNS instruments to run more efficiently and reliably, while opening the potential for future improvements. The largely successful overhauling experience of utilizing open-source and community-driven Control System demonstrates the potential to be widely adopted.

E-mail of the corresponding author: vodopiveck@ornl.gov

Thursday, October 13th 2022, 14:10-14:40

Open Science at Forschungszentrum Jülich (OS4FZJ)

Oliver BERTUCH[2], Torsten BRONGER[2], Dorit JERGER[1], **Sven RANK**[1], Robert SPECK[3]

[1] Forschungszentrum Jülich, Corporate Development, Jülich, Germany

[2] Forschungszentrum Jülich, Central Library, Jülich, Germany

[3] Forschungszentrum Jülich, Jülich Supercomputing Centre, Jülich, Germany

The open science movement has come a long way – in several meanings of the phrase. Firstly, it has evolved and expanded over about two decades to now incorporate a growing variety of open practices in data management, software engineering, access to publications, transfer and innovation, and several more fields. Secondly, as open science is taking shape as a definable set of practices, organizations are coming to grips with it, i.e., they draw up policies or strategies to foster open science, hire people and set up infrastructure. Thirdly, as the various open practices stand today at different stages of development and evolve at different speeds, it seems to be necessary to identify their overlaps, interfaces, and synergies between them.

At Forschungszentrum Jülich, "central" activities for open science started with the movement towards open access to publications in the 2000s in the central library (ZB). Research data management (RDM) was added in the mid-2010s. In the late 2010s it became clear that such digitalization topics could profit from support by corporate development (UE). Now, in the early 2020s, research software engineering (RSE) has completed the cloverleaf of practices that can be grouped under the open science "label". Therefore, a group of protagonists, founded by Jülich Supercomputing Centre (JSC) as one of the key RSE players on campus, ZB and UE, approached the board of directors with a concept sketch called "OS4FZJ" – and received support to put it into practice. It represents an effort to identify overlaps, interfaces, and synergies between open science practices and to start and synchronize these practices and actors at Jülich (e.g. HiRSE_PS, HMC, NFDI people, institute experts, …).

In terms of scope OS4FZJ is intended as a pilot or as a ramp up for future developments at Jülich. It is based on a (very tentative) analysis of the open science status quo at the Forschungszentrum and of the interplay between open science practices, especially between RDM and RSE. The initiative follows the assumption that scholarly outputs and their evaluation are changing. Future excellence will comprise FAIR and open research software and data plus other open research practices that benefit science and society.

The ZB and JSC will share 2 FTEs to establish the three new roles for networking, monitoring, and research software engineering. Tangible products of the initiative will be a community-driven RSE portal, an open science dashboard as well as an open science forum on which ideas for a sustainable future for OS4FZJ can be discussed.

E-mail of the corresponding author: s.rank@fz-juelich.de

Abstracts

Friday, October 14th 2022

Friday, October 14th 2022, 09:00-09:30

Diagnostics for Macromolecular Structure Determination at Neutron Sources: AUSPEX

Yunyun GAO[1], **Andrea THORN[1]**

[1]Universität Hamburg, Institut für Nanostruktur- und Festkörperphysik, Hamburg, Germany

Structures of biological macromolecules are the key to understanding the processes of life and form the basis for developing new drugs, e.g. against COVID-19. To obtain such molecular structures, the neutron or X-ray diffraction of a crystal is measured, processed and interpreted on a large-scale device. However, for ideal use, reliable automatic data analysis software is also needed that gives users direct feedback on the measurement as well as data processing. Early indication of data quality would help to curtail measurement at neutron sources, where single-crystal macromolecular diffraction experiments can be rather time-consuming. Correct background estimation is vital, as weak sources and strong incoherent scattering lead to a low signal-to-background ratio. In addition, neutron experiments use a larger bandwidth of longer wavelengths, which makes standard X-ray integration software such as XDS difficult to use without further adaption. As neutron data collection is still very much limited by the weak sources and availability of dedicated instruments, it is crucial that even weak data can be used to best advantage.
We are looking to implement such a software – AUSPEX [1] - for users at neutron, synchrotron and XFEL source both on-site and as a publicly accessible web service as well as to define new 'best practices' for the measurement at large facilities. As a first step, we have analysed all publicly available neutron data sets in a big-data approach with AUSPEX.

1] Thorn, A.*, Parkhurst, J.M., Emsley, P., Nicholls, R., Evans, G., Vollmar, M. & Murshudov, G.N. (2017) AUSPEX: a graphical tool for X-ray diffraction data analysis, Acta Cryst D73, 729-737.

E-mail of the corresponding author: andrea.thorn@uni-hamburg.de

Friday, October 14th 2022, 09:30-09:50

Single crystal neutron diffraction data reduction with OpenHKL

Zamaan RAZA[1], Christian TRAGESER[1], Ammar NEJATI[1], Andreas OSTERMANN[2], Tobias SCHRADER[1], Joachim WUTTKE[1]

[1]Jülich Centre for Neutron Science (JCNS), Lichtenbergerstr. 1, 85747 Garching, Germany

[2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergerstr. 1, 85747 Garching, Germany

Data reduction is a crucial prerequisite to data analysis in neutron scattering experiments; in the case of single crystal diffraction, it involves the reduction of a set of images at fixed sample rotation increments to a set of Miller indices and detector coordinates. However, the available mature software solutions for this problem are either legacy codes, converted from X-ray diffraction, or are closed-source.

OpenHKL [1] (formerly NSXTool) is a standalone program, currently under development, with a modern graphical user interface that facilitates the data reduction workflow: locating detector spots in the images, indexing them, predicting peaks, refining unit cell parameters and instrument states, integrating the peaks and finally merging them. It is written in C++ for excellent speed, is open-source and well documented, natively handles neutron diffraction experiments with different detector geometries, and has a convenient Python scripting interface.

In this presentation I will demonstrate the capabilities of NSXTool and describe the progress of the project over the past three years.

[1] https://jugit.fz-juelich.de/mlz/openhkl

E-mail of the corresponding author: z.raza@fz-juelich.de

Friday, October 14th 2022, 09:50-10:10

Simplifying diffraction data analysis with EasyDiffraction

Andrew SAZONOV[1], Simon WARD[1] and Piotr ROZYCZKO[1]

[1]European Spallation Source ERIC, P.O. Box 176, SE-221 00, Lund, Sweden

Diffraction is a key tool for structure analysis. However, currently available software for modelling and analysis of diffraction data may be, on the one hand, difficult for new users looking to apply diffraction to their field of expertise and, on the other hand, not flexible enough for domain experts.

EasyDiffraction [1] aims to lower the barrier of entry to diffraction data analysis by providing an intuitive and user-friendly graphical interface, which is distributed as an all-in-one package that includes all dependencies and can be installed with just a few clicks on different operating systems. For more complex problems and increased flexibility the Python library behind EasyDiffraction can be used through Jupyter notebooks and scripting.

Simple interface of EasyDiffraction can help improve the user experience and thereby make it easier to train users and students, as well as be better prepared for experiments. We plan to integrate EasyDiffraction into the full data processing workflow to increase experiment automation and make better use of beam time.

EasyDiffraction is built on the EasyScience framework [2], a platform aimed at unifying neutron scattering analysis software. In addition to diffraction, this framework has been successfully applied to reflectometry. Quasielastic neutron scattering will also be targeted in the future.

Currently EasyDiffraction has the basic features of CrysPy [3] and CrysFML [4] crystallographic libraries. We are collaborating with LLB and ILL regarding the CrysPy and CrysFML, respectively, and more functionality will become available as the project matures.

EasyDiffraction is being developed free and open source, keeping the idea of FAIR and sustainable software in mind. We hope to attract interested people to jointly contribute to this project and help us, for the benefit of everyone, in making diffraction data analysis and modelling easier.

[1] https://easydiffraction.org
[2] https://easyscience.software
[3] https://github.com/ikibalin/cryspy
[4] https://code.ill.fr/scientific-software/crysfml

E-mail of the corresponding author: andrew.sazonov@ess.eu

Friday, October 14th 2022, 10:10-10:30

Efficient data extraction with automated report generation for neutron spin echo raw data

Olaf HOLDERER[1], Piotr ZOLNIERCZUK[2], Stefano PASINI[1], Tadeusz Kozielewski[3], Laura STINGACIU[2], Michael MONKENBUSCH[3]

[1]Forschungszentrum Jülich GmbH, JCNS at MLZ, Garching, Germany

[2]Oak Ridge National Laboratory, NScD, Oak Ridge, USA

[3]Forschungszentrum Jülich GmbH, JCNS, Jülich, Germany

Neutron spin-echo spectrometers with a position-sensitive detector typically map a large range of wavevectors and Fourier times, either combining different wavelength settings at a continuous source or at a pulsed source due to the time-of-flight tagged wavelength frame. Extracting all the information contained in the raw data and mapping them to a suitable physical space in the most efficient way is a challenge. Here we present the workflow of the DrSpine (data reduction for spin echo) software [1], which allows to reduce data from time-of-flight and continuous neutron spin echo instruments and provides a comprehensive report including a preliminary data evaluation for a first assessment of the experimental data.

[1] P. Zolnierczuk, O. Holderer, S. Pasini, T. Kozielewski, L.R. Stingaciu, M. Monkenbusch, Journal of Applied Crystallography, **52**, doi: 10.1107/S1600576719010847 (2019).

E-mail of the corresponding author: o.holderer@fz-juelich.de

Friday, October 14th 2022, 11:00-11:30

Fusing HPC and Edge – Making optimum use of knowledge

Michael BUSSMANN

Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

At the Helmholtz International Beamline for Extreme Fields (HIBEF) located at the European XFEL systems under extreme conditions are studied. These systems are far from equilibrium and most often in a transient state during investigation.
Although we can have atomic temporal and spatial resolution using the high brightness of the European XFEL the complex phase space properties are not easy to resolve. Here, large scale simulations can partially help, although they are expensive and time consuming. With the help of AI we can bring down this effort to a more reasonable scale and try to fuse forward simulations with solving the non-convex inverse problem of retaining information about the systems we study. I will give an overview of state of the art and discuss current developments towards fast inversion of experimental data.

E-mail of the corresponding author: m.bussmann@hzdr.de

Friday, October 14th 2022, 11:30-11:50

Monte Carlo ray tracing simulations for comparison to neutron scattering experiments

G.E. GRANROTH[1], J.Y.Y. Lin[2], F. Islam[3], T. Huegle[3], L. DeBeer-Schmitt[1], A. M. dos Santos[1], M. Guthrie[1], W. Zhou[4], P. Willendrup[5]

[1]Neutron Scattering Division

[2]Second Target Station Project

[3]Neutron Technology Division

[4]Computer Science and Mathematics Division (Oak Ridge National Laboratory, Oak Ridge, Tennessee USA)

[5]Department of Physics (Technical University of Denmark, Denmark)

Monte Carlo Ray tracing simulations are very effective tools for the design of neutron scattering instruments. However, long calculation times and the large body of expertise needed to run the simulations, mean these tools are rarely used to elucidate experimental results. The largest computational resource is usually required by the incident beamline part of the simulation. The GPU support available in McStas 3.X and an NVIDIA A100 processor has allowed this constraint to be overcome for the GPSANS, SNAP, ARCS, and SEQUOIA instruments at Oak Ridge National Laboratory. More specifically, incident beam simulations can be run on the same time scale of, if not faster than, a typical experimental data collection. To reduce the required expertise for the end user to run the simulation, a workflow is being developed that will automatically run an incident beam simulation when a data collection is started on the instrument. A second workflow will allow the use of that simulation in a McVine based sample scattering simulation by providing the run number. The user will be required to use their detailed knowledge of the sample to describe it using a set of XML based files. Current progress and results from these workflows will be summarized.

This work is sponsored through Oak Ridge National Laboratory's Directors Research and Development Fund.

E-mail of the corresponding author: granrothge@ornl.gov

Friday, October 14th 2022, 11:50-12:10

MJOLNIR: Data treatment of CAMEA-like multiplexing instruments

Jakob LASS[1], Daniel G. MAZZONE[1]

[1]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen, Switzerland

Modern massive triple-axis multiplexing spectrometers are increasingly more complex than the standard triple-axis instruments the neutron spectroscopy community has been used in the past. The complexity of performing experiments is shifting from the actual acquisition part during the beamtime towards challenges in data visualization, treatment, and simulation. Thus, understanding the instrument to a detail where it can be modeled with high fidelity is very important in the data evaluation process, as this allows distinguishing between instrumental artefacts, resolution effects and the intrinsic contributions from the sample.

Many novel multiplexing neutron spectrometers employing the CAMEA [1] (Continuous Angle Multi-Energy Analysis) concept are currently being build or already in operation. In the most abstract form, the spectrometer can be reduced to a series of analyzers and detectors - even in the cases where the prismatic concept is employed [2] - and the initial version of our software MJOLNIR [2] is based on this concept. While the philosophy is sufficient for initial data treatment we learned that an in-depth data treatment of specific multiplexing instruments can be achieved only through more detailed information. In this talk I will present our recent computational progress on multiplexing instruments, taking CAMEA at PSI as a model example. Notably, I will report on our recent developments to apply a non-parametric background estimation algorithm and to perform resolution calculations that are accurate for multiplexing spectrometers and based on the Gaussian approximations from Eckold & Sobolev [4].

[1] F. Groitl, D. Graf, J. O. Birk, M. Markó, M. Bartkowiak, U. Filges, C. Niedermayer, C. Rüegg, H. M. Rønnow, *Review of Scientific Instruments*, *87*(3). (2016).
[2] J. O. Birk, M. Markó, P. G. Freeman, J. Jacobsen, R. L. Hansen, N. B. Christensen, C. Niedermayer,M. Månsson, H. M. Rønnow, K. Lefmann. *Review of Scientific Instruments*, *85*(11) (2014)
[3] J. Lass, H. Jacobsen, D. G. Mazzone, K. Lefmann. *SoftwareX*, *12*, 100600. (2020)
[4] G. Eckold, O. Sobolev. *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, *752*, 54–64. (2014)

E-mail of the corresponding author: Jakob.lass@psi.ch

Friday, October 14th 2022, 12:10-12:30

Euphonic: efficient inelastic neutron scattering simulations and more from force constants

Rebecca FAIR[1], Adam JACKSON[2], David VONESHEN[3], Dominik JOCHYM[2], Duc LE[1], Keith REFSON[1], Toby PERRING[1]

[1]ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxfordshire OX11 0QX, UK

[2]Scientific Computing Department, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxfordshire OX11 0QX, UK

[3]Department of Physics, Royal Holloway University of London, Egham, TW20 0EX, UK

Chopper spectrometers produce large 4-dimensional inelastic neutron scattering (INS) datasets, allowing investigations of vibrational and magnetic properties of materials over large regions of momentum-energy (**Q**-E) space. While software (e.g. Horace [1]) exist to enable visualisation and analysis of such data, computational challenges remain for the simulation and fitting of vibrational spectra, which requires the calculation of phonon frequencies and displacements at hundreds of thousands of **Q**-points to simulate a single 2D slice of data. Here we present Euphonic [2], a Python package designed to efficiently interpolate phonons and calculate INS intensities directly from force constants. It has a user-friendly API to allow it to interface with other software, enabling fast and easy simulation of INS intensities directly in Horace, for example. It also has a focus on performance, with key components written in C and OpenMP. The performance scaling of Euphonic means that, for example, instrument resolution convolved simulations of phonon spectra are now tractable for the first time. The API also makes Euphonic useful as a library to the wider scientific community – in addition to being used as a force constants importer or phonon calculator, Euphonic can be used to calculate and plot band structures, density of states and powder averaged coherent INS spectra, with command line tools provided for each case. Currently supported are CASTEP and Phonopy force constants, with the potential for more to be added in the future. Euphonic has been developed following software development best practice, is open-source under the GNU General Public License and can be obtained via Github, PyPI and the conda-forge Conda channel.

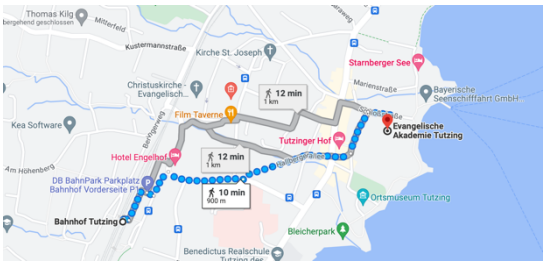
[1] R.A. Ewings, A. Buts, M. D. Le, J. van Duijn, I.Bustinduy and T.G.Perring, *Nucl. Instrum. Methods Phys. Res., Sect. A*, **834**, 132-142 (2016)
[2] R. L. Fair, A. J. Jackson, J. C. King, M. D. Le, C. Pettitt, K. Refson, G. S. Tucker and D. J. Voneshen, Euphonic (2022), DOI: 10.5286/SOFTWARE/EUPHONIC

E-mail of the corresponding author: rebecca.fair@stfc.ac.uk

Location and Accommodation

The workshop venue is the ideally-located Conference Center of the Evangelische Akademie Tutzing, situated directly on Lake Starnberg in the foothills of the Alps, approximately 40km south of Munich.

The workshop fee includes accommodation for 3 nights (11-14 October) in single rooms, fullboard and the workshop dinner.



How to reach Tutzing

From the center of Munich (approx. 50 minutes)

• At Munich main station take the S6 (leaves every 20 minutes) in the direction of Tutzing.
• From the S-Bahn station in Tutzing it is within 10 min walking to the Evangelische Akademie at the lake Starnberg.

From Munich airport (approx. 90 minutes)

• If your flight ticket does not include a journey in the MVV area, your journey with the S-Bahn (city train) to Tutzing requires a day ticket for tariff-zones M-5 (M, 1, 2, 3, 4, 5)
• Take the S1 (leaves every 20 min) in the direction of Munich Hauptbahnhof (main station) as far as Laim station (approx. 40 minutes)
• At Laim change trains at the same platform for the S6 to Tutzing.
• The Evangelische Akademie is approx. 10 min walking distance from the S-Bahn station (Bahnhof) Tutzing at the lake Starnberg. You can find information on the train or bus schedule at the webpage of the Munich Public Transportation Service

http://www.mvv-muenchen.de/en/homepage/index.html

or the Deutsche Bahn service

http://www.bahn.de/

The Organizing committee

Monika Krug
Franziska Michel
Ramona Schurek
Dorothea Henkel (IT Support)
Paulo Innocente (IT-Support)
and Stefano Pasini

Excursion and conference dinner

Thursday, 13th October 2022, 15:00h

A bus will take us from the Conference Centre “Evangelische Akademie Tutzing” to Buchheim to the **Buchheim Museum of Phantasy**, where we will be guided through the exhibitions of the museum.

The Buchheim Museum of Phantasy houses a collection of famous expressionists with works by Erich Heckel, Emil Nolde, Ernst Ludwig Kirchner, Max Pechstein and others. The museum is also a folk and ethnological museum and displays objects collected by Lothar-Günther Buchheim during his travels. Buchheim's own works are also on display.

Buchheim Museum
Am Hirschgarten 1
82347 Bernried
Phone: +49 8158 99700
info@buchheimmuseum.de
www.buchheimmuseum.de

Conference Dinner

After the guided museum tour, we will reach the Restaurant “Hotel Seeblick”, that is located few minutes’ walk from the museum, for our conference dinner at 18:00h.

Hotel Seeblick-
Tutzinger Straße 9
82347 Bernried
Phone: +49 8158-2540#
info@seeblick-bernried.de
www.seeblick-bernried.de

The bus will pick up us approximately 21:00h to take us back to the “Evangelische Akademie Tutzing”.

Firstname	Familyname	Institut
Mois I.	Aroyo	University of Basque Country
Stefanos	Athanasopoulos	European Spallation Source
Nikolaos	Biniskos	Forschungszentrum Jülich GmbH
Georg	Brandl	Forschungszentrum Jülich GmbH
Thomas	Brückel	Forschungszentrum Jülich GmbH
Michael	Bussmann	Helmholtz-Zentrum Dresden-Rossendorf
Jos	Cooper	ISIS neutron and muon source
Jeffrey	Donatelli	Lawrence Berkeley National Lab
Michael	Drüing	Advanced UniByte GmbH
Rebecca	Fair	STFC
Christian	Felder	Forschungszentrum Jülich GmbH
Stephan	Förster	Forschungszentrum Jülich GmbH
Marina	Ganeva	Forschungszentrum Jülich GmbH
Artur	Glavic	Paul Scherrer Institut
Garrett	Granroth	Oak Ridge National Laboratory
Gerrit	Günther	Helmholtz-Zentrum Berlin
Thomas	Gutberlet	Forschungszentrum Jülich GmbH
Moritz	Hannemann	Forschungszentrum Jülich GmbH
Eva M.	Herzig	Universität Bayreuth
Alexander	Hexemer	Lawrence Berkeley National Lab
Michael	Hofmann	TU München
Olaf	Holderer	Forschungszentrum Jülich
Konstantin	Kholostov	Forschungszentrum Jüllich
Petr	Konik	Forschungszentrum Jülich GmbH
Oleksandr	Koshchii	Forschungszentrum Jülich GmbH
Alexandros	Koutsioumpas	Forschungszentrum Jülich GmbH
Jakob	Lass	Paul Scherrer Institute
Duc	Le	STFC
Kuangdai	Leng	Scientific Computing Dept
Klaus	Lieutenant	Forschungszentrum Jülich GmbH
Michael	Linke	Advanced UniByte GmbH
Zhanwen	Ma	Forschungszentrum Jülich GmbH
Anders	Markvardsen	UK Research and Innovation
Tyler	Martin	NIST
Stefan	Mattauch	Forschungszentrum Jülich GmbH
Andrew	McCluskey	European Spallation Source
Yannick	Meinerzhagen	RWTH Aachen University
Martin	Meven	RWTH Aachen University
Osca Mwongera	Mukiri	Forschungszentrum Jülich GmbH
Paolo	Mutti	Institut Laue-Langevin
Noah	Nachtigall	RWTH Aachen University
Ammar	Nejati	Forschungszentrum Jülich GmbH
Stefano	Pasini	Forschungszentrum Jülich GmbH
Brian Richard	Pauw	Bundesanstalt für Materialforschung
Toby	Perring	ISIS Neutron and Muon Source
Aurel	Radulescu	Forschungszentrum Jülich GmbH
Sven	Rank	Forschungszentrum Jülich GmbH

Zamaan	Raza	Forschungszentrum Jülich GmbH
Florian	Rhiem	Forschungszentrum Jülich GmbH
Jose	Robledo	Forschungszentrum Jülich GmbH
Andrew	Sazonov	European Spallation Source
Nicolai	Schmid	Advanced UniByte GmbH
Norberto	Schmidt	Forschungszentrum Jülich GmbH
Astrid	Schneidewind	Forschungszentrum Jülich GmbH
Fabian	Schuelzle	Advanced UniByte GmbH
Abdullah	Shehada	Tomsk Polytechnic University
Michal	Stekiel	Forschungszentrum Jülich GmbH
Mikhail	Svechnikov	Forschungszentrum Jülich GmbH
Mario	Teixeira Parente	Forschungszentrum Jülich GmbH
Andrea	Thorn	Universität Hamburg
Christian	Trageser	Forschungszentrum Jülich GmbH
Gregory	Tucker	European Spallation Source
Guido	Vehres	Forschungszentrum Jülich GmbH
Egor	Vezhlev	Forschungszentrum Jülich GmbH
Nicolò	Violini	Forschungszentrum Jülich GmbH
Klemen	Vodopivec	Oak Ridge National Laboratory
Jörg	Voigt	Forschungszentrum Jülich GmbH
Michael	Wagener	Forschungszentrum Jülich GmbH
Simon	Ward	European Spallation Source
Frank	Weber	Karlsruhe Institute for Technology
Thomas	White	DESY
Joachim	Wuttke	Forschungszentrum Jülich GmbH
Jianhui	Xu	RWTH Aachen University