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ORNL/TM-2025/3772

Report on the "Symposium on Advancements in Simulating Neutron Scattering Instruments and Experiments"

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Marshall McDonnell
Martin Mourigal
Paolo Mutti
Matthew Tucker
Christoph Wildgruber
Peter Willendrup

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October 29-30,2024

OAK RIDGE National Laboratory

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Neutron Technology Division

REPORT ON THE "SYMPOSIUM ON ADVANCEMENTS IN SIMULATING NEUTRON SCATTERING INSTRUMENTS AND EXPERIMENTS"

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October 29-30,2024

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831
managed by
UT-BATTELLE LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

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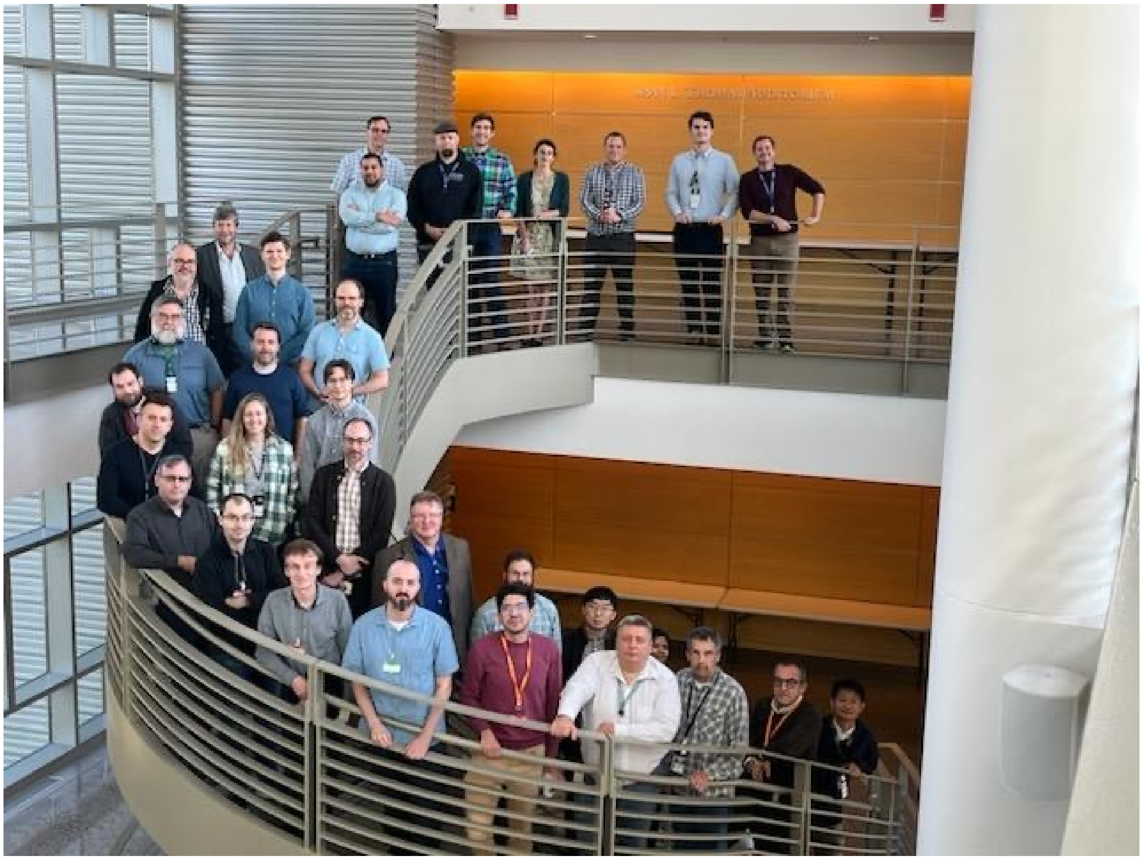

1 Executive Summary

An international group of researchers gathered for the "Symposium on Advancements in Simulating Neutron Scattering Instruments and Experiments" at Oak Ridge National Laboratory (ORNL) on October 29-30, 2024. The symposium highlighted state-of-the-art advancements in neutron scattering instrument simulations and the development of digital twins for scattering instruments.

This document summarizes the recurring themes from the 19 talks and discussions. A key focus was on the role of neutronics simulations in the design, analysis, and performance optimization of neutron instruments. Presentations featured the most widely used software packages, such as McStas, McVine, Vitess, and MCNP.

Another major theme addressed the analysis and interpretation of experimental neutron data, where materials models and simulations play a critical role. Talks on relevant software tools, including NCrystal, OCLimax, and Paradyse, were delivered by their respective developers.

During the symposium, both talks and breakout sessions explored strategies to enhance the interplay between neutronics simulations and materials models. A key question emerged: How can we develop a Real-Time Explainable Digital Twin of a neutron scattering experiment? Discussions include the idea that the Digital Twin concept has implications for instrument control and testing.

Through this symposium, we gained valuable insights into the challenges and requirements for developing a Real-Time Explainable Digital Twin of a neutron scattering experiment. The discussions and presentations paved the way for future innovations in this rapidly advancing field.

Advanced neutron scattering instrument and experiment simulation are providing unique capabilities:
new insights in:

Analysis and Support Materials :- Simulations are becoming an integral part of neutron scattering experiments, enhancing data analysis by allowing direct comparisons between experimental and simulated results. Monte Carlo Ray Tracing methods, such as McStas and MCViNE, are now capable of leveraging GPU acceleration, making simulations up to 1000 times faster. This enables near real-time analysis, ensuring that experiments can be adjusted dynamically. Additionally, user-friendly interfaces, such as Calvera, streamline simulation workflows by automating data input and processing, making advanced modeling tools accessible to a broader scientific community.
Training :- The use of digital twins and virtual experiments is transforming the way researchers prepare for neutron scattering experiments. By integrating simulation tools directly into instrument control systems, researchers can perform realistic practice runs before actual beam time. This significantly reduces errors, improves efficiency, and maximizes the scientific return from each experiment. Facilities like MLZ are implementing simulation-driven training programs, ensuring that users are well-prepared and can optimize instrument settings before conducting physical measurements.
Setting optimization and making decision :- Advanced simulation tools are playing a crucial role in optimizing neutron beamlines, guiding critical design decisions. Studies on neutron optics, such as guide systems, beam divergence control, and chopper configurations, help fine-tune instruments to achieve higher neutron flux and improved resolution. Machine learning and computational optimization techniques are being incorporated to evaluate thousands of possible configurations, leading to faster and more precise instrument adjustments. These developments ensure that neutron facilities operate at peak efficiency, delivering the best possible experimental conditions for researchers.
Bridging Simulations and Experiments: Workflow Advancements :- A major challenge in neutron scattering is ensuring that simulations align closely with real experimental conditions. The concept of real-time experimental steering, enabled by digital twins, allows scientists to dynamically adjust experiments based on live data feedback. This integration of simulations into experimental workflows enhances reproducibility, improves measurement accuracy, and reduces uncertainty. Emerging AI-driven techniques, such as automated data reduction pipelines and predictive modeling, are further strengthening the connection between simulated and experimental neutron scattering studies, paving the way for fully autonomous experiment optimization.

2 Review of Talks

Each invited talk given in the workshop is summarized below. The talks covered a broad range of topics, and are grouped below by corresponding science/technical area.

2.1 Analysis and support materials

2.1.1 "Monte Carlo Ray Tracing simulations for comparison to data." Garrett Granroth, ORNL

The focus of this talk was on the applications of Monte Carlo Ray Tracing methods to analyze data acquired on samples on neutron instruments. Four major points were given.

1. Experiments should run near or at the speed of the beamline measurement.
2. Simplified input for the user
3. Use each Monte Carlo Ray tracing Code for its optimal purpose
4. Couple as much of this together in a workflow engine.

To point one both McStas[1] and MCViNE[2, 3] now include GPU enabled code. For McStas it was shows that speed increases of 200 - 1000 times can be realized by using a single commodity GPU card for incident beam simulations of the ARCS, GPSANS, and SNAP Instruments at ORNL. Similar speed ups can be realized for sample simulations using GPUs in MCViNE.

To ease input for the user we calculate incident beam simulations based on acquired data nexus files. That way the user only has to think about the details of the sample configuration. These simulations are performed using Mcstas to leverage the GPUs and the well tested nature of McStas for these applications.

The problems where Monte Carlo ray tracing is particularly useful for analysis is where complex multiple scattering is observed. Say examples of multiple scattering in the sample[4], sample environment[5], or both. MCViNE is ideally suited to this case with it's ability to combine multiple scatters and multiple scattering kernels in each. This functionality has been well tested.

Finally, to provide an interface for the users and to wrap these codes together, we have been using Calvera which is a web based interface that leverages the Galaxy workflow tool. Here a user provides a nexus file to run an incident beam simulation. Then with that incident beam simulation and the xml sample assembly files the samples simulation is run. It provides an output in a neXus file of the same format as the data and then can be compared to the measured data directly. By precalculating the incident beam the sample simulation can be iterated on if a sample parameter is changed or to find an relevant sample parameter. In summary Calvera abstracts the intricate technical details, allowing users to focus on interpreting results and making data-driven decisions without needing extensive expertise in simulation methodologies.

Expansion to other instruments is envisioned. Specifically a project to include Nomad and disordered simulations is underway.

Much of this work has been funded by the Laboratory Directors' Research and Development fund at ORNL Through the NDIP, MCU, and NeuMatix projects.

[1] Peter Kjær Willendrup and Kim Lefmann. "McStas (ii): An overview of components, their use, and advice for user contributions". In: *Journal of Neutron Research* 23 (2021), pp. 7–27. DOI: 10.3233/JNR-200186.

[2] Jiao YY Lin et al. “MCViNE–An object oriented Monte Carlo neutron ray tracing simulation package”. In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 810 (2016), pp. 86–99.
[3] Coleman J. Kendrick, Jiao Y. Y. Lin, and Garrett E. Granroth. “Using Numba for GPU acceleration of Neutron Beamline Digital Twins”. In: *Proceedings of the 22nd Python in Science Conference*. Ed. by Meghann Agarwal, Chris Calloway, and Dillon Niederhut. 2023, pp. 46–52. DOI: 10.25080/gerudo-f2bc6f59-006.
[4] JYY Lin et al. “Using Monte Carlo ray tracing simulations to model the quantum harmonic oscillator modes observed in uranium nitride”. In: *Physical Review B* 89.14 (2014), p. 144302.
[5] J. L. Niedziela et al. “Design and operating characteristic of a vacuum furnace for time-of-flight inelastic neutron scattering measurements”. In: *Review of Scientific Instruments* 88.10 (Oct. 2017), p. 105116. ISSN: 0034-6748. DOI: 10.1063/1.5007089. eprint: https://pubs.aip.org/aip/rsi/article-pdf/doi/10.1063/1.5007089/16132150/105116_1_online.pdf. URL: https://doi.org/10.1063/1.5007089.

2.1.2 "Modeling neutron scattering experiments on quantum materials using semiclassical spin dynamics and ray-tracing simulation." Martin Mourigal, Georgia Tech

The presentation explores advancements in modeling neutron scattering experiments, particularly focusing on quantum materials. It begins with challenges in quantum magnetism and the complexities of lattice-based spin systems, highlighting the Heisenberg model and its role in neutron scattering studies. High-fidelity simulations using semiclassical spin dynamics and tools like Sunny.jl are presented, demonstrating their application to real-world experiments, such as on HYSPEC, and studies on spin-S pyrochlore magnets. The integration of digital twins to enhance instrument precision and streamline experimental workflows is emphasized, along with future needs such as resolution-informed multi-sampling, background corrections, and improved interfaces. The talk concludes by envisioning next-generation instruments, incorporating advanced crystal analyzers and extreme experimental conditions, while stressing user-centric design and collaboration to push the boundaries of neutron scattering research.

2.2 Advancement in software

2.2.1 "An overview of NCrystal - a library for modeling of thermal neutron interactions " Thomas Kittelmann, ESS

The presentation introduces NCrystal, an open-source library designed for simulating thermal neutron transport, initially created to enhance Geant4 simulations with accurate modeling of crystalline materials. NCrystal provides robust tools for thermal neutron scattering, featuring support for various material types (crystals, liquids, amorphous solids) and advanced physics algorithms, such as Bragg diffraction, inelastic scattering, and multiphase materials. It is compatible with multiple Monte Carlo simulation frameworks like McStas and OpenMC, and its flexible configuration enables integration across platforms. The library leverages formats like NCMAT for material definitions and provides Python APIs and CLI tools for accessibility. NCrystal emphasizes computational efficiency, achieving high speeds in simulations and material initialization. Recent updates include features for small-angle neutron scattering (SANS) and capabilities for expanding vibrational density of states (VDOS) into scattering kernels on-the-fly, enhancing its application in neutron science and simulation workflows. The project continues to evolve, supported by collaborations and grants, aiming to improve neutron scattering realism and usability.

2.2.2 "Status report and news from the McStas team." Peter Willendrup, ESS

The presentation provides a comprehensive overview of McStas, a Monte Carlo neutron ray-tracing simulation software. It begins with an introduction to the software's historical development, core functionality, and its critical role in neutron scattering experiments. Key highlights include McStas's flexibility, user-friendly interface, and its application in designing, optimizing, and troubleshooting neutron instruments, such as those at the European Spallation Source (ESS) and Oak Ridge National Laboratory (ORNL). The slides discuss McStas's extensive library of components, enabling researchers to simulate complex experimental setups with high precision. The presentation emphasizes recent updates, such as the integration of McStas with Python-based tools like McStasScript, which allows for automated workflows, parameter studies, and advanced data visualization. It also highlights the use of Union components for modeling intricate beamline setups, including multi-instrument configurations and detailed sample environments. These advancements, validated through experimental benchmarking, enhance the software's accuracy and reliability. The presentation concludes with a focus on future directions, aiming to make McStas even more versatile and aligned with cutting-edge scientific requirements.

2.2.3 "Code extensions to MCNP for highly detailed radiation transport calculations of neutron beamlines." Kyle Grammer, ORNL

There are a number of challenges to modelling detailed radiation transport for a neutron beamline with an eye towards estimating and then mitigating instrument backgrounds. The standard code tool for these calculations is MCNP [**werner_mcnp_2018**], which is a general purpose radiation transport tool. The instrument designers produce quite detailed models of neutron beamlines in McStas and it is important for this detail to also be propagated to MCNP. The tool McStas2CAD is used to generate a CAD compatible conversion of an individual McStas instrument and the Geomwriter tool [1] processes this from multiple instruments along with other CAD or CSG (such as from GEOUNED [2]) inputs into a detailed CSG model of the instruments and the facility for radiation transport and shielding calculations. This streamlines the model generation in MCNP from weeks or months to less than 1 day.

MCNP lacks a number of features that are important for simulating neutron beamlines. Several new tools have been developed to perform these more detailed calculations using MCNP. The neutron supermirror extension [3, 4] allows the propagation of neutrons from the moderator to the instrument end station via an empirical guide reflectivity function without requiring the use of multiple codes and secondary sources at various locations along the beamline. The supermirror extension has been upgraded to estimate the capture of neutrons in the supermirror layer as well as polarization from a supermirror v-cavity. The rotating objects extension [5] provides the ability to simulate a rotating object, such as a chopper or velocity selector, which includes the neutron absorption in the spinning object and the transmitted beam in a single calculation. The single crystal [6] extension adds an oriented material functionality for simulating monochromators or single crystal filters. The SANS extension [7] adds a new scattering process and the ability to simulate fine powder materials, such as filters that are used to smear out phase space at the exit of a guide. The gravity extension [8] calculates neutron trajectories along parabolic trajectories, which has a strong effect on the deflection of cold neutrons in free flight as well as the detailed phase space of neutrons propagating through a long neutron guide system. Finally, the NCrystal extension allows the user to call NCrystal for the determination of the scattering cross section and the handling of the scattering process rather than MCNP and cross section libraries and kernels.

The combination of these detailed models and physics extensions to MCNP provide an avenue for rapid turn-around of MCNP model calculations as well as the ability to investigate instrument backgrounds.

[1] Kyle Grammer. *GEOMWRITER - A WORKFLOW FOR AUTOMATICALLY GENERATING MCNP GEOMETRY FOR NEUTRON GUIDE SIMULATIONS*. English. Tech. rep. ORNL/TM-2022/2397. Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States), Feb. 2023. DOI: 10.2172/2305830. URL: https://www.osti.gov/biblio/2305830 (visited on 02/21/2024).

[2] J.P. Catalán et al. “GEOUNED: A new conversion tool from CAD to Monte Carlo geometry”. In: *Nuclear Engineering and Technology* (2024). ISSN: 1738-5733. DOI: https://doi.org/10.1016/j.net.2024.01.052.

[3] F X Gallmeier et al. “Implementation of Neutron Mirror Modeling Capability into MCNPX and Its Demonstration in First Applications”. In: *Nuclear Technology* 168.3 (Dec. 2009), pp. 768–772. DOI: 10.13182/NT09-A9304. URL: https://www.tandfonline.com/doi/full/10.13182/NT09-A9304.

[4] M. Magán and Ryan M. Bergmann. “Supermirror physics with event biasing in MCNP6”. en. In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 955 (Mar. 2020), p. 163168. ISSN: 0168-9002. DOI: 10.1016/j.nima.2019.163168. URL: https://www.sciencedirect.com/science/article/pii/S0168900219314755 (visited on 02/22/2022).

[5] Kyle B. Grammer, Franz X. Gallmeier, and Erik B. Iverson. “A Chopper Extension to model neutron transport with non-static surfaces and high-speed moving media in MCNPX 2.7”. en. In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 932 (July 2019), pp. 43–49. ISSN: 0168-9002. DOI: 10.1016/j.nima.2019.04.052. URL: https://www.sciencedirect.com/science/article/pii/S0168900219305224 (visited on 11/14/2022).

[6] F. X. Gallmeier et al. “Introducing single-crystal scattering and optical potentials into MCNPX: Predicting neutron emission from a convoluted moderator”. In: *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 814 (2016), pp. 39–49. DOI: 10.1016/j.nima.2015.12.053.

[7] Kyle B. Grammer and Franz X. Gallmeier. “The small-angle neutron scattering extension in MCNPX and the SANS cross section for nanodiamonds”. en. In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 953 (Feb. 2020), p. 163226. ISSN: 0168-9002. DOI: 10.1016/j.nima.2019.163226. URL: https://www.sciencedirect.com/science/article/pii/S0168900219315098 (visited on 11/14/2022).

[8] Kyle B. Grammer. “The gravity extension for MCNP 6.2”. In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 1061 (Apr. 2024), p. 169136. ISSN: 0168-9002. DOI: 10.1016/j.nima.2024.169136. URL: https://www.sciencedirect.com/science/article/pii/S0168900224000627 (visited on 02/19/2024).

2.2.4 "Digital Twins using Vitess: Simulation Control from NICOS." Klaus Lieutenant, JCNS

In the beginning, neutron instrument simulation software was mainly used to optimize instrument designs in terms of high flux and favorable beam properties at the sample position. Then it was extended to virtual experiments by adding sample and detector in the simulation. They are used to check the instrument performance in terms of the final output, to test data evaluation software and to find the best instrument setups for planned real experiments. In a present project at MLZ, we include VITESS instrument simulations in the NICOS operation system that is used to run the real experiments. For the user, a virtual experiment looks exactly like a real experiment. This enables training of users before the beamtime, which - in combination with testing instrument settings - allows a much more efficient use of the beamtime. The goal is to allow changing parameters (like slit sizes, device positions, etc) during the simulation so that a virtual experiment appears like a real experiment and is ideally also as fast. This is realized by reading an interface during the simulation and changing the simulation parameters on the fly. It is currently realized for the reflectometer MARIA, but will be extended to other instruments, until all MLZ instruments have digital twins for testing and training purposes, either based on VITESS or on McStas simulations. Details of the concept for the parameter change during the simulation were presented.

2.2.5 "Simulating the NMX instrument using Union components and McStasScript." Mads Bertelsen, ESS

This presentation explores the simulation and refinement of the NMX macromolecular crystallography instrument at the European Spallation Source (ESS) using advanced tools like McStasScript and Union components. The NMX instrument is tailored for protein crystallography with neutrons, particularly for studying hydrogen locations in large biological molecules. Initial simulations, created for the instrument proposal, have evolved to support operational needs such as calibration, diagnostics, and full experiments in sample environments.

McStasScript, a Python-based interface for McStas, simplifies the creation and execution of simulations, providing features like parameter management, visualization, and metadata handling. The integration of Union components allows for enhanced modeling of beamline elements, detectors, and sample environments with greater realism. Examples include constructing detector models and analyzing correlations between simulated and measured data.

The presentation emphasizes adherence to simulation standards at ESS, ensuring consistency and utility for commissioning and operations. It also highlights ongoing efforts to minimize discrepancies between simulations and measurements, addressing issues like misalignments, mirror degradation, and chopper phase errors. Ultimately, this work contributes to a comprehensive library of instrument, sample environment, and sample models, paving the way for improved instrument performance and user experience

2.2.6 "Thermal nuclear data development in support of moderator and reflector simulations" José Ignacio Marquez Damian, ESS

The presentation delves into advancements in the development of thermal neutron scattering data to support simulations for moderator and reflector systems at neutron facilities like ESS. It emphasizes the need for accurate nuclear data to model current systems, such as liquid hydrogen moderators and beryllium reflectors, and to support future upgrades like liquid deuterium moderators and advanced materials, including diamond nanoparticles and clathrate hydrates. Key tools developed include NCrystal, NJOY+NCrystal, and other Monte Carlo simulation methods that integrate molecular dynamics (MD) and density functional theory (DFT) to enhance physics-based scattering models. The presentation highlights significant innovations, such as accounting for crystallite size and texture effects in materials like beryllium and solid methane, implementing spin correlation effects, and extending support for asymmetric scattering kernels. These developments have been benchmarked against experimental data and are freely accessible through repositories like GitHub. The work underscores the importance of integrating advanced simulation tools to optimize neutron instrument performance and accommodate evolving facility needs, positioning these methods as critical for the next generation of neutron science.

2.3 Beam optimization and making decision

2.3.1 "Neutron optics: Exotic guide simulation." Thomas Huegle, ORNL

This presentation explores innovative approaches to neutron guide system design, focusing on optimizing neutron transport for diverse instrument requirements. Starting from basic, unoptimized guide layouts, Thomas Huegle discusses the challenges of accommodating multiple instruments with varying beam needs, such as diffractometers, imaging systems, and small-angle neutron scattering (SANS) setups. Techniques like multichannel benders, tapered "squeezer" guides, and octagonal or squeezed-octagonal geometries are introduced to manage beam divergence and intensity distribution. Novel concepts such as "randomizers" and Bezier-spline-based guides aim to decouple neutron angle and origin correlations for improved phase space control. Challenges in implementation include managing multiple imaging locations, maintaining shielding constraints, and aligning complex parameters like aperture configurations and curved geometries. The presentation highlights the need for creative, parameter-rich solutions to address the unique demands of neutron beamline optimization while balancing practical considerations like cost and shielding limitations

2.3.2 "V-Cavity Optimization and Simulation on the Cold Neutron Spectrometer PoLAR." Leland Harriger, NIST

The presentation discusses the development and optimization of the PoLAR cold neutron spectrometer, focusing on its primary spectrometer components and the application of advanced simulation techniques. Key areas include the optimization of flux at the sample position, achieved through the design of a focusing guide and a dynamic monochromator. The work employs Monte Carlo simulations using McStas to refine performance metrics such as resolution and intensity across a range of incident energies (2.5 to 15 meV). The V-cavity polarizer, an innovative design feature, is optimized to enhance incident polarization, balancing parameters like taper angle and coating to match the guide's divergence and spatial cross-section. Comparisons between single-channel and multi-channel polarizers highlight differences in flux and transmission performance, guiding design decisions. The integration of virtual alignment techniques and Monte Carlo modeling ensures precise instrument configurations, supporting user experiments and expanding PoLAR's capabilities. Future directions include leveraging these tools for continued optimization and alignment with user needs, making PoLAR a versatile platform for neutron scattering research.

2.3.3 "Global optimization of neutron optics from the source to the detector." Christoph U Wildgruber, ORNL

This presentation focuses on the global optimization of neutron optical systems, using a Time-of-Flight Small Angle Neutron Scattering (TOF SANS) instrument concept for the Second Target Station (STS) as a case study. The optimization addresses a multi-objective problem, including maximizing neutron flux on the sample, achieving low $q_{\min}$ values for data collection, and enhancing the instrument's ability to distinguish protein conformations in samples. A 48-parameter McStas model was developed, leveraging Differential Evolution (DE) algorithms to explore the complex parameter space and identify globally optimized configurations. Key findings include the effectiveness of segmented elliptical guides and optimized apertures in reducing instrument length while significantly increasing neutron flux. The study also highlights the importance of balancing flux, resolution, and background control, with sensitivity tests identifying critical parameters like aperture sizes and guide lengths. By incorporating science-driven metrics into the optimization, such as distinguishing protein conformations using scattering data, the workflow demonstrates its potential for designing efficient, versatile neutron instruments. The approach's robustness and efficiency suggest its applicability to broader instrument design challenges, with future directions including GPU-based computations for enhanced performance.

2.3.4 "Utilizing simulations in the development and optimization of neutron beamlines at the MIT Reactor." Sean Fayfar, MIT

The presentation focuses on the development and optimization of neutron beamlines at the MIT Reactor (MITR), particularly the 4DH4 beamline. MITR, a 6 MW light-water-cooled reactor, supports various experimental facilities and operates continuously in 10-week cycles. The main beamline features a polychromatic neutron beam with a bismuth filter and hosts two instruments: a radiography/tomography setup and a multiplexing stress-strain diffractometer. To optimize limited flux and floor space, the team developed a digital twin of the beamline using SIMRES and incorporated bent-perfect silicon crystal analyzers for dispersive imaging. The presentation describes the stepwise construction of the beamline, challenges faced during a prolonged reactor shutdown, and integration of new equipment like He-3 detectors and modern motor controllers. Future plans include transitioning to McStas for simulations and exploring additional instrument concepts, such as single-crystal and powder diffractometers, to expand capabilities. This work demonstrates the importance of simulations and iterative improvements in advancing neutron beamline functionality.

2.3.5 "Alignment of Simulation With Reality: Beam Measurements Towards Better Understanding of Scattering Instrument Capabilities." Matthew J. Frost, ORNL

This presentation by Matthew J. Frost addresses the importance of aligning simulations of neutron scattering instruments with actual beam measurements to enhance their accuracy and applicability. The presentation highlights a systematic approach to refining simulations through direct comparison with measurements and iterative updates. The process involves a detailed characterization process that includes source measurements (e.g., pulse shapes, spectral brightness, and moderator imaging) and instrument measurements (e.g., beam divergence, spectral intensity, and resolution). Examples from instruments such as WAND², VULCAN, and NOMAD demonstrate how specific beam characteristics are measured and used to parameterize simulation inputs, such as guide geometry, source performance, and attenuation effects. This approach enables continuous refinement of scattering capabilities by supporting upgrades, new designs, and enhanced decision-making processes at large-scale neutron facilities.

2.4 Bridging Simulations and Experiments: Workflow Advancements

2.4.1 "Ongoing Journey to Digital Twin and Experimental Steering for Nanoscale-Ordered Materials Diffractometer." Marshall McDonnell, ORNL

This presentation discusses advancements in experimental steering and the development of digital twins for the NOMAD diffractometer at ORNL. Experimental steering involves automating data analysis and decision-making to enable dynamic control of neutron scattering instruments, improving beam time utilization, and automating routine tasks. The presentation highlights ORNL's Neutron Data Interpretation Platform (NDIP) as a central tool for connecting workflows, integrating external computing resources, and enabling secure instrument control via a REST API. Virtual instruments, built using Monte Carlo ray tracing (McStas/McVine) and atomistic simulations, are presented as essential for testing experimental steering workflows before physical execution. Digital twins, defined as interconnected physical and digital models, are proposed for NOMAD to improve experiment forecasting and explore transient phenomena. Tools like NeuMATIX bridge atomistic simulations and instrument simulations to compare experimental and simulation data effectively. The work emphasizes the growing role of automation, data integration, and virtual testing in advancing neutron scattering research, supported by robust workflows and interdisciplinary collaborations.

2.4.2 "Harnessing Digital Twins and Simulation for Advancing Neutron Experimentation." Paolo Mutti, ILL

Data from virtual experiments are becoming a valuable asset for research infrastructures: to develop and optimize current and future instruments, to train in the usage of the instrument control system, to study quantifying and reducing instrumental effects on acquired data. Furthermore large sets of simulated data are also a necessary ingredient for the development of surrogate models (supervised learning) for faster and more accurate simulation, data reduction and analysis. So far, the production and usage of data from virtual experiments have been mostly reserved to simulation experts. In this symposium, he presented how at ILL data from virtual experiments are made available to the general users. The presented framework wraps in a digital twin of the facility instruments, the knowledge of its physical description, the simulation software and the high performing computing setup. The twin presented in this talk has been developed at the ILL in the framework of the PANOSC European project in close collaboration with other research facilities (ESS and EuXFel) for some of its essential components. An overview of the core simulation software (McStas), its Python API (McStasScript), the public instrument description repository and the instrument control system (NOMAD) are given. The choices on the the communication patterns, based on ZQM, and interaction between the different components are also presented. A flavor of advanced features like collision prediction has also been presented.

2.4.3 "Simulations and Data-Driven Approaches for Neutron Vibrational Spectroscopy." Yongqiang Cheng, ORNL

Y.Q. Cheng's presentation highlights the evolving role of digital twin technologies and AI/ML in neutron scattering research. The presentation discusses the challenges of simulating inelastic neutron scattering (INS) spectra, emphasizing the need for computational modeling to interpret experimental data. Tools like OCLIMAX bridge theoretical and experimental approaches, supporting full scattering analysis and interfacing with atomistic modeling and data analysis software. Machine learning force fields (MLFFs) accelerate energy and force calculations compared to traditional density functional theory (DFT), enabling faster simulations for complex systems. Large synthetic INS databases for thousands of molecules and crystals support the training of AI models for real-time predictions, helping researchers without advanced modeling expertise or computing resources. Innovations like symmetry-aware neural networks and latent space representations facilitate direct predictions of $S(Q, E)$ spectra, making simulations more accessible. These novel approaches have be applied to understand and interpret features in INS spectra, including isotope substitution, multiphonon excitations, and anharmonicity. The AI/ML method is particularly suitable for complex material modeling such as TiO-SiO glasses. This work, supported by the U.S. Department of Energy, demonstrates how integrating AI/ML with neutron scattering enables real-time simulations, enhances efficiency, and provides deeper insights into material dynamics.

2.4.4 "Development of data reduction workflows for MLZ instruments TOPAS and POWTEX using Vitess simulations." Oleksandr Koshchii, JCNS

The Heinz Maier-Leibnitz Zentrum (MLZ) in Garching near Munich, built around the FRM-II research reactor, offers its scientific users about 30 instruments for neutron research. Several new instruments are currently being under construction. In particular, a tof spectrometer with polarization analysis TOPAS and a tof diffractometer for POWder and TEXture analysis POWTEX. When both instruments will be ready for operation, it is important that the users can proceed to the data analysis stage shortly after performing their measurements. This means that they should be provided with all the necessary supplemental tools, including those for data reduction. Data reduction is among the most important and time-consuming steps that researchers have work on in order to link raw data collected during a neutron scattering experiment to a meaningful scientific publication. In his presentation, Oleksandr talked about the development of data reduction workflows for TOPAS and texture measurements at POWTEX using realistic instrument simulations in Vitess. The data processing pipeline for TOPAS includes extensive use of Scipp and ScippNeutron Python libraries. For texture measurements at POWTEX, the developed workflow is integrated into a new software called EasyTexture. The graphical user interface of the software is being built using a user-friendly Python/QML framework EasyScience.

APPENDIX A. SUPPLEMENTARY MATERIAL

A.1 Workshop Agenda

Copy of the workshop agenda is shown on the following pages.

Oak Ridge National Laboratory AGENDA

MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

Oak Ridge National Laboratory, Building 8600, C-156
October 29-30, 2024

Day 1 — Oct. 29

Time	Event	Speaker	Moderator
8:00 – 8:30am	Badging and Registration: SNS Lobby (working breakfast) Breakfast is served at RM-150		
8:30 – 8:40am	Welcome Guests to SNS	Richard Ibberson, ORNL	Fahima Islam
8:40 – 8:50am	Symposium Charge	Fahima Islam, ORNL	Fahima Islam
8:50 – 9:30am	"Monte Carlo Ray Tracing simulations for comparison to data"	Garrett Granroth, ORNL	Fahima Islam
9:30 – 10:10am	"An overview of NCrystal - a library for modeling of thermal neutron interactions"	Thomas Kittelmann, ESS	Fahima Islam
10:10– 11:10am	"Status report and news from the McStas team"	Peter Willendrup, ESS	Fahima Islam
10:23 –11:20am	Break		
11:20–12:00pm	"Neutron optics: Exotic guide simulation"	Thomas Huegle, ORNL	Fahima Islam
12:00 – 1:20pm	Working Lunch and presentation:"Potential of Digital Twins for the STS"	Leighton Coates, ORNL	Fahima Islam
1:20 – 2:00pm	"Ongoing Journey to Digital Twin and Experimental Steering for Nanoscale-Ordered Materials Diffractometer"	Marshall McDonnell, ORNL	Matt Frost
2:00 – 2:40pm	"Code extensions to MCNP for highly detailed radiation transport calculations of neutron beamlines"	Kyle Grammer, ORNL	Matt Frost
2:40-3:20 pm	Discussion		
3:20 – 4:00pm	"Digital Twins using Vitess: Simulation Control from NICOS"	Klaus Lieutenant, JCNS	Matt Frost
4:00 – 4:15pm	Break		
4:15 – 4:55pm	"Harnessing Digital Twins and Simulation for Advancing Neutron Experimentation"	Paolo Mutti, ILL	Matt Frost

4:55 - 5:35pm	"Modeling neutron scattering experiments on quantum materials using semiclassical spin dynamics and ray-tracing simulations"	Martin Mourigal, Georgia Tech	Matt Frost
5:35 – 6:30pm	Guided Discussion/Working Dinner Topic: "What do we mean by digital Twin"	Organizing panel(Led by Matt Tucker , ORNL)	

Symposium on Advancements in Simulating Neutron Scattering Instruments and Experiments

Oak Ridge National Laboratory, Building 8600, C-156
October 29-30, 2024

Day 2 — Oct. 30

Time	Event	Speaker	Moderator
8:50 – 9:00am	Introduction to Second Day (Breakfast is served at RM 150)	Thomas Huegle, ORNL	
9:00 – 10:00am	"V-Cavity Optimization and Simulation on the Cold Neutron Spectrometer PoLAR"	Leland Harriger, NIST	Thomas Huegle
10:00 – 10:40am	"Alignment of Simulation with Reality: Beam Measurements Towards Better Understanding of Scattering Instrument Capabilities"	Matt Frost, ORNL	Thomas Huegle
10:40 – 11:20am	"Simulating the NMX instrument using Union components and McStasScript"	Mads Bertelsen, ESS	Thomas Huegle
11:20 – 11:35am	Break		
11:35am – 12:15pm	"Global optimization of neutron optics from the source to the detector"	Christoph U Wildgruber, ORNL	Thomas Huegle
12:15 – 1:30pm	Working lunch presentation: 'Neutron Scattering Simulations for User Programs"	Jon Taylor, ORNL	A.J. (Timmy) Ramirez-Cuesta
1:30 – 2:10pm	"Thermal nuclear data development in support of moderator and reflector simulations"	José Ignacio Marquez Damian, ESS	A.J. (Timmy) Ramirez-Cuesta
2:10 – 2:50pm	Discussion		

2:50 – 3:50 pm	"Simulations and Data-Driven Approaches for Neutron Vibrational Spectroscopy"	Yongqiang Cheng, ORNL	A.J. (Timmy) Ramirez-Cuesta
3:50-4:05 pm	Break		
4:05 – 4:45pm	"Utilizing simulations in the development and optimization of neutron beamlines at the MIT Reactor."	Sean Fayfar, MIT	A.J. (Timmy) Ramirez-Cuesta
4:45 - 5:25pm	"Development of data reduction workflows for MLZ instruments TOPAS and POWTEX using Vitess simulations"	Oleksandr Koshchii, JCNS	A.J. (Timmy) Ramirez-Cuesta
5:25 – 6:30pm	Guided Discussion/ Working Dinner Topic: "Where we are in virtual neutron scattering simulation"	Organizing Panel (led by Garrett Granroth)	