

Symposium on Advancements in Simulating Neutron Scattering Instruments and Experiments

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)		
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 analysis of mixed samples”	Garrett Granroth, ORNL	Fahima Islam
9:30 – 10:10am	“An overview of NCrystal - a library for modeling of thermal neutron interactions”	Thomas Kittlemen, ESS	Fahima Islam
10:10– 11:10am	“Status report and news from the McStas team”	Peter Willendrup, ESS	Fahima Islam
11:10 –11:20am	Break		
11:20–12:00pm	“Neutron optics: Exotic guide simulation”	Thomas Huegle, ORNL	Fahima Islam
12:00 – 1:20pm	Working lunch presentation: ‘Neutron Scattering Simulations for User Programs’	Jon Taylor, ORNL	Fahima Islam
1:20 – 2:00pm	“Ongoing Journey to Digital Twin and Experimental Steering for Nanoscale-Ordered Materials Diffractometer”	Marshall McDonel, 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 Vitesse: 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		Martin Mourigal, Georgia Tech	Matt Frost
5:35 – 6:30pm	Guided Discussion/ Working Dinner Topic: “Where we are in virtual neutron scattering simulation”	Organizing Panel (led by Garrett Granroth)	

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Day 2 — Oct. 30

Time	Event	Speaker	Moderator
8:50 – 9:00am	Introduction to Second Day	Thomas Huegle, ORNL	
9:00 – 10:00am	“A General Approach to Virtual Single Crystal and Instrument Alignment in McStas”	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 – 11:30am	Break		
11:30am – 12:10pm	“Global optimization of neutron optics from the source to the detector”	Christoph U Wildgruber, ORNL	Thomas Huegle
12:10 – 1:30pm	Working Lunch and presentation: “Potential of Digital Twins for the STS”	Leighton Coates, ORNL	A.J. (Timmy) Ramirez-Cue sta
1:30 – 2:10pm	“Thermal nuclear data development in support of moderator and reflector simulations”	José Ignacio Marquez Damian, ESS	A.J. (Timmy) Ramirez-Cue sta

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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-Cue sta
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	Fahima Islam
4:45 - 5:25pm	“Development of data reduction workflows for MLZ instruments TOPAS and POWTEX using Vitess simulations”	Oleksandr Koshchii, JCNS	Fahima Islam
5:25 – 6:30pm	Guided Discussion/Working Dinner Topic: “What do we mean by digital Twin”	Organizing panel(Led by Matt Tucker , ORNL)	