



Machine Learning for Synchrotron and Neutron Scattering Workshop

Hybrid: In person at the Advanced Light Source and virtually via Zoom

April 17 - April 18, 2023

Morning Session: 8am - 12:30pm

Afternoon Session: 1:30pm - 5:00pm

8:15 am	Welcome Session Chairs: Eric Roberts & Tanny Chavez	Alex Hexemer, Stephan Roth, Peter Zwart, and James Sethian
8:30 am	Machine Learning: History, Now and Future <i>(25 minutes + 5 minutes discussion)</i>	Wiebke Köpp
9:00 am	Title: Use of machine learning, artificial intelligence and robotics at the Heinz Maier-Leibnitz Zentrum (MLZ) <i>(20 minutes + 5 minutes discussion)</i>	Peter Müller-Buschbaum
9:25 am	Title: HPC+AI@Edge Enabled X-ray Science <i>(20 minutes + 5 minutes discussion)</i>	Mathew Cherukara
9:50 am	Title: Classification of SAS patterns using ML on transformed 2D data <i>(30 minutes + 5 minutes discussion)</i>	Marina Ganeva and Stephan Förster
10:25 am	Break	
10:40 am	Title: The NIST Autonomous Formulation Laboratory: A.I. Driven Formulation Discovery and Optimization <i>(20 minutes + 5 minutes discussion)</i>	Tyler Martin

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10:55 am	Title: Adaptively driven XRD measurements for autonomous phase identification <i>(20 minutes + 5 minutes discussion)</i>	Nathan Szymanski
11:20 am	Discussion Panel (ML at Facilities) <i>Köpp, Müller-Buschbaum, Cherukara, Ganeva, Förster, Martin, Nathan Szymanski</i>	
12:30 pm	Lunch: Working Lunch Chairs: Grace Luo & Wiebke Köpp	
1:30 pm	Title: Active learning-assisted neutron spectroscopy with log-Gaussian processes <i>(20 minutes + 5 minutes discussion)</i>	Mario Teixeira Parente
1:55 pm	Title: Faster and lower dose X-ray measurements enabled by physics-informed machine learning <i>(20 minutes + 5 minutes discussion)</i>	Stefan Kowarik
2:20 pm	Talk: AI and Machine Learning aided prompt analysis of powder diffraction and PDF data <i>(20 min + 5min discussion)</i>	Simon Billinge
2:45 pm	<i>Break (15 minutes)</i>	
3:00 pm	Title: Combining model-based simulation and machine learning for GISAXS analysis <i>(20 minutes + 5 minutes discussion)</i>	Stephan Roth
3:25 pm	Title: Advanced Gaussian Process Function Approximation and Uncertainty Quantification for Autonomous Experimentation <i>(20 minutes + 5 minutes discussion)</i>	Marcus Noack
3:50 pm	Title: Bits and Atoms: Exploring the Intersection of Machine Learning and Microscopy	Maxim Ziatdinov
4:15pm	Panel Discussion (Autonomous Experiments) <i>Parente, Kowarik, Billinge, Roth, Noack, Ziatnidov</i>	
	5:00 pm, end of day 1; Dinner on your own	

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Date: April 18th

Morning Session: 8:30am - 12:30 pm

Afternoon Session: 1:30pm - 3:55 pm

Session Chairs: Zhuowen Zhao & Tibbers Hao

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| 8:30 am | Unlocking the Power of Machine Learning in Scientific User Facilities: An introduction to MLEExchange
<i>(20 minutes + 5 minutes discussion)</i> | Tanny Chavez |
| 8:55 am | Title:
<i>(20 minutes + 5 minutes discussion)</i> | Eric Roberts |
| 9:20 am | Title: Lessons learned from X-ray data: microstructure, phases and the role of deep learning
<i>(20 minutes + 5 minutes discussion)</i> | Dani Ushizima |
| 9:45 am | Title: Towards scalable flexible organic-metal interfaces: unraveling the structure-property-relation of functional and doped P3HT-based thin films using ML-enhanced data analysis.
<i>(20 minutes + 5 minutes discussion)</i> | Benedikt Sochor |
| 10:10 am | <i>Break (20 minutes)</i> | |
| 10:30 am | Title: AI & ML at Diamond Today and in the Future.
<i>(20 minutes + 5 minutes discussion)</i> | Tim Snow |
| 11:05 am | Title: Machine learning for surface scattering
<i>(30minutes + 5 minutes discussion)</i> | Frank Schreiber and Vladimir Starostin |
| 11:40 pm | Open Discussion (Software and Infrastructure)
<i>(50 minutes)</i> | |
| 12:30 pm | Working Lunch
<i>(1 hour)</i> | |

Session Chairs: Alex Hexemer, Peter Zwart, Stephan Roth

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1:30 pm	Title: <i>(10 minutes + 5 minutes discussion)</i>	Guiseppe Portale
1:45 pm	Title: Closing the Loop <i>(20 minutes + 5 minutes discussion)</i>	Linus Pithan
2:10 pm	Title: <i>(20 minutes + 5min discussion)</i>	Baskar Ganapathysubramanian
2:35 pm	Title: Deploying Machine Learning Based Segmentation for X-ray Diffraction Images at Synchrotron Facilities <i>(20 minute + 5min discussion)</i>	Howard Yanxon
3:00 pm	break	
3:15 pm	DLSIA, or Deep Learning for Scientific Image Analysis <i>(20 minutes discussion)</i>	Eric Roberts
3:35 pm	GISAXS:Simulation of GISAXS Patterns with Non-analytical Form Factors <i>(20 minutes discussion)</i>	Dinesh Kumar
3:55pm	Discussion and Closeout <i>(30 minutes discussion)</i>	

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List of Speakers

23 Total

Name	Affiliation	Participation
Stephan Roth	Deutsches Elektronen-Synchrotron	Onsite
Peter Muller-Buschbaum	Technische Universität München	
Tyler Martin	National Institute of Standards and Technology	
Benedikt Sochor	Deutsches Elektronen-Synchrotron	
Baskar Ganapathysubramanian	Iowa State University	
Mariana Ganeva	Jülich Supercomputing Centre	
Simon Billings	Columbia University	
Tim Snow	Diamond Light Source	
Mathew Cherukara	Argonne National Laboratory	
Frank Schreiber	University of Tübingen	
Gerbrand Ceder	University of California, Berkeley	
James Sethian	University of California, Berkeley	Onsite
Dinesh Kumar	Center for Advanced Mathematics for Energy Research Applications	
Guiseppa Portale	University of Groningen	

External participants = 14

List of Participants

Name	Affiliation	Participation
Peter Zwart	Lawrence Berkeley National Laboratory	Onsite
Alex Hexemer	Lawrence Berkeley National Laboratory	Onsite
Tanny Chavez	Lawrence Berkeley National Laboratory	Onsite
Dani Ushizima	Lawrence Berkeley National Laboratory	Onsite
Angela Setiadi	Lawrence Berkeley National Laboratory	Onsite
Andrea Taylor	Lawrence Berkeley National Laboratory	Onsite
Amanda Espiritu	Lawrence Berkeley National Laboratory	Onsite

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Sheena Ryan	Lawrence Berkeley National Laboratory	Onsite
Heidi Clark	Lawrence Berkeley National Laboratory	Onsite

Internal participants = 9

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