Joint APS/CNM Workshop 1: Leveraging AI and Large Language Models in Scientific User Facilities

Thursday, May 8, Morning

8:30 – 8:45 Workshop Organizers
Welcome and Opening Remarks

8:45 – 9:25 Luca Rebuffi (Advanced Photon Source, Argonne National Laboratory)
AI-driven Automatic Optimization of Nano-focused Beams and Wavefronts

9:25 – 10:05 Alexander Hexemer (Advanced Light Source, Lawrence Berkeley National Laboratory)
Emerging AI Tools and Workflows for Enhanced Scientific Discovery at User Facilities

10:05 – 10:15 Break

10:15 – 10:55 Vivek Thampy (Stanford Synchrotron Radiation Light Source)
AI-driven Discovery of High-performance Ferroelectric Materials for Energy-efficient Microelectronics

10:55 – 11:35 Kibaek Kim (Mathematics and Computer Science, Argonne National Laboratory)
Foundation Model for BCDI and Ptychographic Images

11:35 – 12:15 Apurva Mehta (SLAC National Accelerator Laboratory)
Towards Digital Twins for Risk-averse Control of Multielement Crystal Optics

12:15 – 1:30 Lunch Break

Thursday, May 8, Afternoon

1:30 – 2:10 Esther Tsai (Center for Functional Nanomaterials, Brookhaven National Laboratory)
Towards AI-embedded X-ray Scattering Experimentation

2:10 – 2:50 Chris Lu (OpenAI)
Towards Using AI for Fully Automated Open-ended Research

2:50 – 3:30 Daniil A. Boiko (Department of Chemical Engineering, Carnegie Mellon University)
LLM Agents in Chemical Sciences: Where Can We Get More Data?

3:30 – 3:40 Break

3:40 – 5:30 Xiangyu Yin (Argonne National Laboratory)
Empowering X-ray Science with Foundation Models and Agentic Workflow

Tutorial 1: LLM Assistants for Extracting and Organizing Scientific Data

1. *Overview of tools and techniques for leveraging LLMs to streamline data extraction and organization.*
2. *Hands-on exercises using real-world scientific datasets.*

Break

Tutorial 2: LLM Assistants for Experiment Workflow and Operation

1. *Demonstrating how LLMs can assist in planning, optimizing, and automating experimental workflows.*
2. *Interactive session with practical examples and simulations.*

5:30 Workshop Organizers
Closing Remarks and Networking Opportunity

5:35 Adjourn