

## Explainable AI for the Sciences: Towards Novel Insights

**Monday January 9, 2023**

- 8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*
- 9:00 *Session Chair: Tulay Adali*
- 9:00–9:50 **Bolei Zhou** (University of California, Los Angeles (UCLA))  
*From Network Dissection to Policy Dissection: Discovering Emergent Concepts in Deep Representations*
- 10:00–10:15 *Break*
- 10:15–11:05 **Klaus-Robert Müller** (Technische Universität Berlin)  
*Virtual Talk:*
- 11:15–11:30 *Break*
- 11:30–12:20 **Xiao Fu** (Oregon State University)  
*Understanding Multiview and Self-Supervised Representation Learning: A Nonlinear Mixture Identification Perspective*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Jaesik Choi** (Korea Advanced Institute of Science and Technology (KAIST))  
*Explainable Artificial Intelligence to Analyze Internal Decision Mechanism of Deep Neural Networks*
- 3:30–3:50 *Break*
- 3:50–4:40 **Bin Yu** (University of California, Berkeley (UC Berkeley))  
*Virtual Talk: Interpreting Deep Neural Networks towards Trustworthiness*
- 4:45–5:20 *Lightning Poster Session*
- 5:20–6:30 *Poster Session & Reception (Hosted by IPAM)*

**Tuesday January 10, 2023**

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *SESSION CHAIR: Michele Ceriotti*
- 9:00–9:50 **Osbert Bastani** (University of Pennsylvania)  
*Interpretable Machine Learning via Program Synthesis*
- 10:00–10:15 *Break*

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- 10:15–11:05 **Wojciech Samek** (Fraunhofer Institute for Telecommunications, Heinrich Hertz Institute, HHI)  
*Virtual Talk: Concept-Level Explainable AI*
- 11:15–11:30 *Break*
- 11:30–12:20 **Tülay Adalı** (University of Maryland Baltimore County)  
*Matrix and Tensor Factorizations for Data Fusion: Focus on Model Match, Interpretability, and Reproducibility*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Frederick Klauschen** (Ludwig-Maximilians-Universität München)  
*AI in cancer research and diagnostics*

### Wednesday January 11, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *SESSION CHAIR: Pamela Douglas*
- 9:00–9:50 **Evrin Acar** (Simula Research Laboratory)  
*Virtual Talk: Extracting Insights from Complex Data: Constrained Multimodal Data Mining using Coupled Matrix and Tensor Factorizations*
- 10:00–10:15 *Break*
- 10:15–11:05 **Michele Ceriotti** (École Polytechnique Fédérale de Lausanne (EPFL))  
*Physical insights from atomic-scale machine learning*
- 11:15–11:30 *Break*
- 11:30–12:20 **Cecilia Clementi** (Freie Universität Berlin)  
*Efficient algorithms for Non-Local Filtering and applications to Cryo-Electron microscopy and biological microscopy*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Petros Koumoutsakos** (Harvard University)  
*Alloys of Artificial Intelligence and Scientific Computing for Fluid Mechanics*
- 3:30–3:50 *Break*
- 3:50–4:40 **Gregoire Montavon** (Freie Universität Berlin)  
*Virtual Talk: Towards Higher-Order and Disentangled Explainable AI*

## Thursday January 12, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:50 **André Freitas** (University of Manchester)  
*Building explanation machines for science: a neuro-symbolic perspective*
- 10:00–10:15 *Break*
- 10:15–11:05 **Matteo Valleriani** (Technische Universität Berlin)  
*XAI Historian*
- 11:15–11:30 *Break*
- 11:30–12:20 **Oliver Eberle** (Technische Universität Berlin)  
*Explainable structured machine learning in similarity, graph and transformer models.*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Anders Søgaard** (University of Copenhagen)  
*What's Opaque to Whom - and Why?*
- 3:30–3:50 *Break*
- 3:50–4:40 *Panel Discussion*

## Friday January 13, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Vince Calhoun** (Georgia Institute of Technology)  
*Title not available*
- 10:00–10:15 *Break*
- 10:15–11:05 **Pamela Douglas** (UCLA Medical School)  
*TBA*
- 11:15–11:30 *Break*
- 11:30–12:20 **Nikolaus Kriegeskorte** (Columbia University)  
*Controversial stimuli: Optimizing experiments to adjudicate among computational hypotheses*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Lisa Nickerson** (Harvard Medical School)  
*Addressing Confounds in Neuroimaging Machine Learning Predictions*

