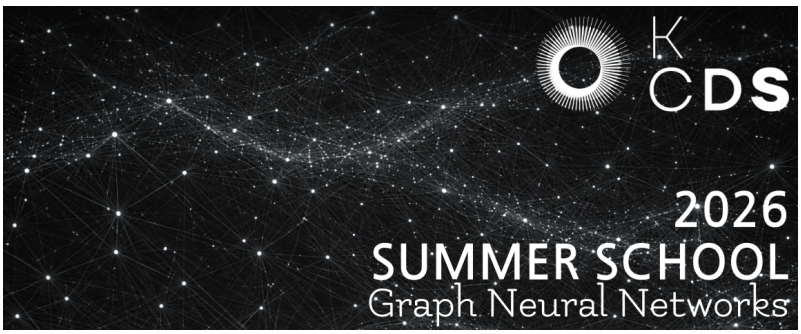
KCDS Summer School 2026



Monday, September 21, 2026 - Friday, September 25, 2026

KIT Geb 20.30

Scientific Program

Jan Stühmer is the head of the research group Machine Learning and Artificial Intelligence (MLI) at Heidelberg Institute of Theoretical Studies (HITS). He is also Junior professor at the Karlsruhe Institute of Technology (KIT). He will give an introduction to geometric deep learning, its theoretical foundations and core concepts, and in the following tutorial we will learn how to apply these concepts in practice. In a second part he will present applications of geometric deep learning in our research: We will discuss applications in protein design and materials science, learn how to fix the order bias in large language models, and discuss our latest research results on approximate equivariance.

Ismail Ilkan Ceylan is an Associate Professor at TU Vienna and an Adjunct Principal Investigator at AITHYRA with extensive expertise in graph machine learning. His long-term goal is to develop reliable and robust learning systems capable of reasoning over relational patterns across diverse domains. We are thrilled to welcome him to teach a course on graph transformers and graph foundation models.

Petar Veličković is a Senior Staff Research Scientist at Google DeepMind and Affiliated Lecturer at the University of Cambridge. A distinguished figure in geometric deep learning, his work has been central to its development and widespread adoption. Currently, his research focuses on aligning neural networks to computation to assess andimprove their reasoning andextrapolation capabilities.We are thrilled to welcomehim to give an online lectureat our summer school!

Joel Oskarsson is a post-doctoral fellow at the ETH Zurich AI Center. His research focuses on machine learning for spatio-temporal modeling in general and applications to earth science in particular. In his course he will give us an introduction to modeling the complex correlations that govern observations across space and time is a central scientific challenge. We will see how GNNs, often combined with other neural network architectures, can be used to model and forecast complex spatio-temporal systems. One domain where such GNNs are effectively applied is Earth system modeling, where they can help us predict future weather or understand climate dynamics. We will cover foundational concepts in machine learning for Earth science, before diving into recent advances in graph-based weather models.

Arghya Bhowmik is an Associate Professor at the Technical University of Denmark (DTU). His research focusses on how we model, search, and design molecules and materials. In his lectures, we will explore how graph neural networks and geometric deep learning can represent atomic structures and act as fast surrogate models for high-accuracy atomistic simulations. We will furthermore discuss graph representation-based generative inverse models for molecules and materials, including how learned chemical and structural representations can guide discovery across vast design spaces. In his hands-on session we will explore how to build practical data-driven workflows using foundation models, surrogate simulations, and automated screening tools for materials and molecule discovery.